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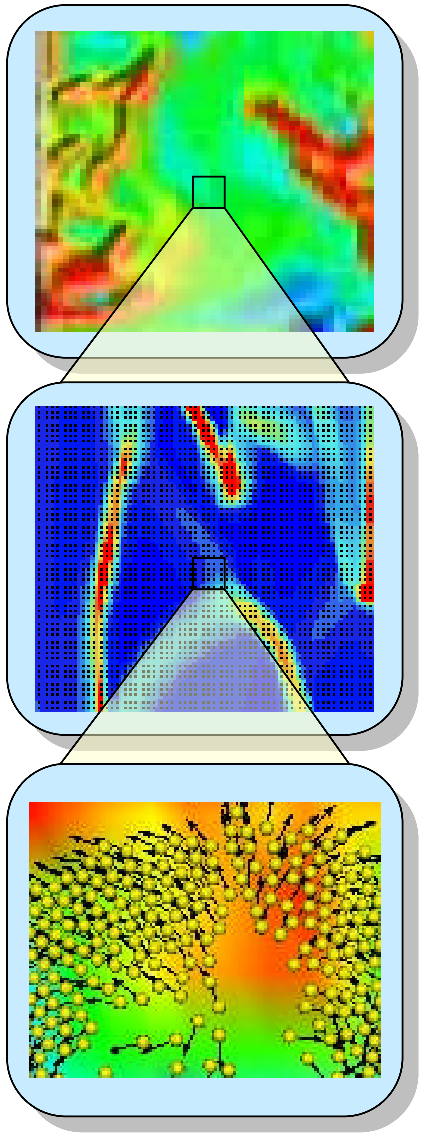
Report on Workshop on Multiphase Flow Research, Morgantown, WV, June 6-7, 2006



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U.S. Department of Energy. Office of Fossil Energy
National Energy Technology Laboratory

Cover Graphics: The simulation results show a description of gas-solids flow at three scales. The simulations at finer scales can be used for formulating constitutive relations for the coarser scales. The coarser simulations are computationally faster and, hence, more suitable for the practical simulation of industrial reactors. The top picture shows large-scale structures in a circulating fluidized bed calculated using a coarse-grained continuum model (device scale). The red color indicates regions where the solids concentration is high and blue indicates low solids concentration. The middle picture shows clusters calculated using a continuum model (meso scale). The fine computational grid superimposed on the picture is only barely discernible. The bottom picture shows particle motion around a bubble in a fluidized bed calculated using a discrete element model (micro scale). The particles and their velocity vectors are shown. All the calculations were performed using NETL's MFIX code. M. Syamlal, NETL.

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Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation. Advances in computing and connectivity make it possible to develop computational models and capture and analyze unprecedented amounts of experimental and observational data to address problems previously deemed intractable or beyond imagination. Yet, despite the great opportunities and needs, universities and the Federal government have not effectively recognized the strategic significance of computational science in either their organizational structures or their research and educational planning. These inadequacies compromise U.S. scientific leadership, economic competitiveness, and national security.

— Principal finding in PITAC Report *Computational Science: Ensuring America's Competitiveness*, June 2005

In the past century, scientific research has been extraordinarily successful in identifying the fundamental physical laws that govern our material world. At the same time, the advances promised by these discoveries have not been fully realized, because the real-world systems governed by these physical laws are extraordinarily complex. Computer-based simulation provides a means of solving the mathematical equations and predicting the behavior of complex systems that can only be described empirically at present.

—*Scientific Discovery through Advanced Computing*

About This Report

This report is the result of a workshop on multiphase flow research held at the National Energy Technology Laboratory, Morgantown, West Virginia, on June 6-7, 2006. The workshop was sponsored by Dr. Robert Romanosky, Technology Manager for Power Systems Advanced Research at NETL. It was attended by 62 researchers from universities, industry, national labs, NASA, and NSF. The discussions were organized into four technical tracks, and the technical track discussions were led by a chairperson from industry, a co-chairperson from a university, and an NETL representative. This report is a compilation of reports written by track chairs based on information discussed at the meeting and obtained from researchers that could not attend the meeting or from other sources. The primary purpose of the report is to look ahead as to what is needed to achieve the workshop goal and not to comprehensively review what has been done. So any review presented is not meant to be complete. All the workshop participants were given the opportunity to review and comment on the report before it was released. Ultimately, the information in the report is the view of the experts that wrote the different sections of this report. The names of the authors appear at the end of each section.

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3. Liquid-solids and gas-liquid flows	P. Ma	R. Fox	I. Gamwo
4. Computational physics and applications	R. Cocco	C. Hrenya	C. Guenther

Report Editor: M. Syamlal

Summary

On June 6-7, 2006, 62 researchers from universities (24), industry (20), national labs (14), NASA (3), and NSF (1) met at the National Energy Technology Laboratory (NETL), Morgantown, WV, to discuss outstanding research problems in multiphase flow with particular relevance to energy technologies and to chart out a roadmap for solving such problems. The vision of the workshop was to "ensure that by 2015 multiphase science-based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants." The discussions were organized into four technical tracks: (1) Dense gas-solids flows and granular flows, (2) Dilute gas-solids flows, (3) Liquid-solids and gas-liquid flows, and (4) Computational physics and applications. The technical track discussions were led by a chairperson from industry, a co-chairperson from a university, and an NETL representative. Pre-workshop technical discussions were facilitated through the workshop website. At the workshop, the technical discussions started with an opening presentation from each technical track. This was followed by four parallel technical track breakout sessions where the topics were discussed by groups of around 15 people. On the second day, the findings of the breakout sessions were discussed in general sessions; the topics were first grouped by the technical tracks and then by overarching themes.

Multiphase flow is prevalent in fossil fuel processes, appearing in the form of gas-solids, gas-liquid, and gas-liquid-solids systems. These systems are notoriously difficult to design and scale up. The volume fraction of different phases can vary from low to high within a short length scale. The flows invariably span multiple time and length scales and pose enormous computational and experimental challenges. For example, the granular flow in a fluidized bed may range from incompressible to hypersonic, while the granular media may undergo a phase change similar to a gas-to-solid transition, all within the same reactor. The volume fraction, stress, and energy typically fluctuate spatially and temporally with amplitudes comparable to the mean. The interaction of the phases with boundaries is often complex and poorly understood. Because multiphase flows may not exhibit a clear separation among the spatial and temporal micro-, meso-, and macro- scales, advanced multi-scale theories may be needed to analyze them.

There was general agreement that achieving the workshop vision, therefore, is a critical and timely need, considering the challenges

involved in building highly efficient, near-zero emission fossil energy plants in the next 20 years. Addressing the challenges involved in new power generation in the United States only would lead to great economic benefits. If the applications to worldwide power generation and to chemical, petroleum, mineral, consumer products, and pharmaceuticals industries are considered, the potential economic benefit is enormous.

Computer Simulations

At the outset, it became clear that the envisioned **computational fluid dynamic (CFD) simulations** would require a set of software tools, not one tool, for several reasons. First, there is a need for a hierarchy of models based on different levels of details, which in the order of decreasing levels of details are direct numerical simulation (DNS), discrete element modeling (DEM), continuum model, coarse-grained continuum model, and various reduced order models. For industrial applications it may be possible to use only coarse-grained continuum models (for design) or reduced order models (for process simulation and control), and the more detailed models (DNS, DEM, and continuum) are necessary for validating or for generating closures for the less detailed models. Second, although desirable, it is not certain that the same software can be used for describing different types of flows (gas-solids, gas-liquid, gas-liquid-solids) or even for different flow regimes within a particular type of flow (dense and dilute in gas-solids flow; bubbly flow, plug flow, stratified flow, and slug regimes in gas-liquid flow). Third, there are different numerical techniques such as finite volume, finite element, volume of fluid, and Lattice Boltzmann that need to be explored. Fourth, the distribution of the models could be an open or closed source. Open source software is necessary for facilitating peer review and promoting scientific advances. Commercial (often closed source) software is preferred by industry because of the availability of user support and consulting services. Also the deployment must be staged so that the industry gets usable software tools (not fully accurate) early on while the university and national lab researchers are continually refining the tools. Finally, there is a need for several preprocessing tools for setting up simulations and postprocessing tools for analyzing, visualizing, and "data mining" output results.

While there is no need for all of the above software tools to be subsumed in monolithic software, researchers need the capability to compose novel hybrid or multiscale models or new applications by linking different software tools: 1) link multiphase flow models at different levels of details (e.g., DEM with continuum model); or 2) link multiphase models with models that consider other physical phenomena (e.g., stress analysis) or larger physical systems (e.g., process simulation). Therefore, the software tools are best developed as components with well-defined interfaces that can be linked using framework software.

There is a need for a standard set of simulation cases (based on analytical solutions and physical and numerical experimental data) that can be used by university and commercial software developers to verify (that the mathematical model is expressed and solved correctly by the software) and validate (that the mathematical model correctly describes reality) computational software.

The desired turnaround time of computer simulations was determined to be about nine hours, so that the simulation results can be routinely used for design. Certain benchmark industrial problems (e.g., coal gasifier) need to be specified. The workshop vision would be achieved if such problems in 3D, including chemical reactions, can be solved to a desired degree of accuracy in less than nine hours.

Theory

Computational software is an embodiment of the underlying **theory**. To achieve the workshop vision, several key theoretical questions need to be solved.

Key near-term questions in dense gas-solids flows and granular flows pertain to the stresses: What defines the stress for the relevant flow regimes? How is stress transmitted throughout the material? How are these related to boundary conditions, particle properties, and process control parameters? What is the character of fluctuations that occur in stresses/forces and flow fields? A near- to mid-term need is the handling of the transition from flows in which the particles are in enduring contact to flows in which the particles are in collisional contact.

A near-term need is the development of constitutive relations that can handle particle size and density distributions, invariably found in industrial reactors. Models are needed for the drag and stresses (e.g., multi-particle kinetic theories).

Gas-solids flows often give rise to particle clustering that significantly affects the macroscopic flow characteristics. It is important to know how particle clustering affects fluid flow structure at different scales and how particles interact with turbulent eddies of different length and time scales.

How do instabilities lead to fluctuations in concentration and how do the clusters affect the drag, collisions, and turbulence modulation?

A near-term need is to ensure that the models correctly capture the effect of temperature and pressure.

A near- to mid-term challenge is accurately modeling gas-liquid flow regime transitions; e.g., the transition in a bubble column from "bubbly" to "churn turbulent" regime. Also there is a need to formulate meso-scale models to bridge the gap between micro and macro-scale phenomena. There is a need to consider the effect of lubrication forces in particle-particle interactions.

A near- to mid-term need is the formulation of proper boundary conditions. The treatment of inlets and outlets and wall boundary conditions must be addressed. The wall boundary condition must capture key effects such as the solids flux distribution near a wall. DEM was recognized as a powerful tool for generating data that can be used to develop and validate wall boundary conditions.

A mid- to long-term need is to model particle deposition and re-suspension, which includes the effect of particle size distribution. A mid-term need is the development of constitutive models for non-spherical particles. A mid- to long-term need is the description of chemical reactions that involve non-spherical particles.

A mid- to long-term need is to understand the effect of electrostatic and particle surface forces (cohesion). It remains to be determined whether electrostatics is important at process temperatures encountered in fossil fuel reactors. A related need is to demonstrate that the models are correctly able to predict the transition in the fluidization behavior when the particle properties change from Geldart group B to group A. Another mid- to long-term need is the development of models that can correctly model the effect of internals, such as heat transfer tubes.

A few mid- to long-term needs are the ability to model particle attrition and agglomeration, fragmentation of coal, particle dispersion in fuel injectors and gasifiers, effect of gases generated by coal on the fluid dynamics, radiation from wall and particles, and refractory erosion.

A long-term need is solving several fundamental theoretical challenges in mathematical formulations of multiphase flow: satisfactory resolution of ill-posedness of continuum multiphase flow equations, eliminating the need to time-average the solution of continuum models for statistically steady problems. What level of mathematical representation is needed in both continuum and discrete particle approaches to enable one to capture physical phenomena? The multiphase turbulence models must consistently incorporate fluctuations in the volume fraction.

Experiments

Experiments ultimately determine the validity of the theory and the computer simulations. Three types of experiments were identified. The first includes experiments used for measuring relevant physical and transport properties, interphase correlations, and chemical reaction rates. The second includes lab and pilot-scale experiments used for studying physical phenomena or industrial reactors. These experiments are usually conducted not with model validation as the objective; their main objective is to generate engineering data needed for designing devices and processes. It was recommended that modelers should be involved in the design of these types of experiments to ensure that the physical properties and boundary conditions needed for setting up computer simulations are measured, and the data become useful for model validation as well.

The third includes experiments specifically designed to test different aspects of theory. This type of experiment is not commonly conducted and is very much needed. For example, well-defined single particle experiments may provide insight into modeling multi-particle systems. These experiments could be physical as well as numerical (e.g., DEM or DNS). There is a need to define a hierarchy of such standard experiments that can be used to validate models.

There is a need to define relevant material properties for different flow regimes (e.g., collisional parameters, internal angle of friction, etc.), develop efficient ways to represent properties in models, and establish standards for material properties and methods.

A near-term need is a drag law applicable over the entire range of solids volume fraction. Despite many attempts, it appears that no way exists to develop an accurate, universal drag law for a poly-dispersed powder. A possible path would be to develop standardized experiments, detailed simulations (discrete element or lattice Boltzmann), or a combination of both from which custom drag formulas could be developed for a given powder.

There is a need to develop well-calibrated, non-intrusive probes and to simultaneously measure the velocity and volume fraction of different phases. Planar flow fields rather than point-to-point traverses are required (e.g., measure radial solids concentration in a riser using MRI). Also it is important to measure solids and gas velocities and turbulence using a combination of PIV and laser sheet methods in very dilute gas-solids flow.

A near-term need is a measurement of near-wall phenomena. A near- to mid- term need is the measurement of the effect of particle size distribution (PSD); e.g., binary mixture – lateral distribution of particle types and segregation, continuous PSD – measure spatial variation of PSD. A near-to mid-term need is a well-characterized, multiphase chemical reactor with detailed measurements (e.g., ozone decomposition). Another need is to develop measurement techniques for high pressure and temperature bubble columns. Also detailed data given by 3D tomography (MRI, X-ray, capacitance imaging etc.) are needed.

A mid- to long-term need is full-field visualization of rotational motions of spherical and non-spherical particles in quasi-2-dimensional situations and 3D tracking of particles in semi-dilute situations (volume fractions of up to 10 or 15%) that take into account frictional interactions, bidisperse or polydisperse grains, and non-spherical grains.

A long-term need is to provide detailed circulating fluidized bed data on at least 2 scales (~0.15 m and ~0.6 m). The experiments must be well-characterized with well-defined entrance, exit, and boundary conditions. These experiments should report detailed data for local pressure, velocity of solids and gas, solids fraction, fluctuations, cluster sizes, and solids flux.

Collaboration and Education

It was felt that the funding for research in this area is declining, despite the national importance of such research, and the number of engineers trained in this area is decreasing. **Collaboration** is essential to improve the visibility of this research area and to leverage limited resources. A proposed collaboratory should enable collaboration among universities, industry, and national labs, act as a resource center for experimental data and software, undertake outreach activities to industry, and promote research driven by industrial needs. **Education** of the next generation of engineers in this area should also be facilitated by the collaboratory.

♦ M. *Syamlal, S. Sundaresan, D. Gidaspow*

FutureGen, the Integrated Sequestration and Hydrogen Research Initiative, is a $1 billion industry/government partnership to design, build and operate a coal gasification-based, nearly emission-free, coal-fired electricity and hydrogen production plant. The 275-megawatt prototype plant will serve as a large scale engineering laboratory for testing new clean power, carbon capture, and coal-to-hydrogen technologies. It will be the cleanest fossil fuel-fired power plant in the world. Virtually every aspect of the prototype plant will employ cutting-edge technology. With respect to sequestration technologies, captured CO_2 will be separated from the hydrogen perhaps by novel membranes currently under development. It would then be permanently sequestered in a geologic formation. Candidate reservoir(s) could include depleted oil and gas reservoirs, unmineable coal seams, deep saline aquifers, and basalt formations - all common in the United States. www.netl.doe.gov/technologies/coalpower/futuregen/index.html

Introduction

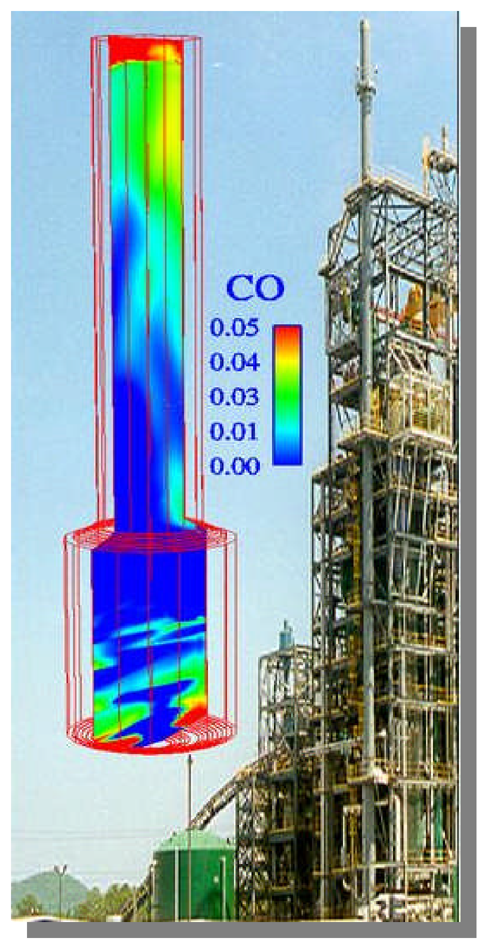
The objective of the workshop was to discuss the development of computational multiphase flow capabilities so that computer simulations can be used for the design, troubleshooting, and operation of devices in advanced fossil fuel plants. The expectation was that the workshop would result in a technical roadmap showing the way to achieve that vision through the collaborative effort of researchers from across the nation. This report fulfills the first part of that expectation.

In the next several paragraphs we will discuss why the above vision is important from an NETL and fossil energy perspective. Furthermore, it is well known that understanding and simulating multiphase flows is of critical national importance. We will briefly discuss that standpoint as well.

Many NETL and advanced fossil energy technologies use complex solids-based reactors whose design needs to be improved to meet the efficiency, reliability, and pollutant reduction targets of future power plants. Solids constitute a major feedstock in NETL technologies; e.g., coal, petroleum coke, biomass, black liquor, oil shale. Solids also appear as sorbents in hot gas cleanup systems or as catalysts in shift converters. Most NETL technologies, from the existing ones to those being considered for the future, involve one or more solids processing steps; e.g., coal gasification and combustion, shale oil extraction, chemical looping, oxy-combustion, oxygen-free gasification, direct reduction of iron ore. Three of the four barrier issues for the development of advanced fossil fuel technologies identified by NETL are related to solids-based systems. For example, reliability is the single most important technical limitation to be overcome in order to achieve widespread deployment of gasification technology [1], and problems with solids-based systems are prevalent in that technology. Gasifier feed injectors are considered to be the weakest links in the technology [1]. Startup problems at the Piñon Pine project are attributable to fines handling and undesirable temperature ramp up in the gasifier [2]. Scale up of solids handling reactors is notoriously difficult [3], which perhaps manifested at Tampa Electric project as lower than expected carbon conversion [2].

Most of the solids-based processes include a carrier gas or liquid and involve chemical reactions as, for example, the burning of coal particles in a stream of air. Solids are often handled in fossil fuel plants using dense and dilute gas-solids flows. In addition, gas-liquid flows and gas-liquid-solids flows also occur in fossil fuel processing; e.g., CO_2 capture and sequestration, shale oil extraction, Fischer-Tropsch reactor, coal-slurry feeder, slurry bubble column reactors, hydrocyclones, trickle bed reactors, absorbers, and scrubbers. Many of these flows occur in combination with homogeneous and heterogeneous chemical reactions. The DTI in the United Kingdom reviewed the status of multiphase flow technology in coal-fired power plants and found that "a lack of basic understanding of particle–fluid interaction, insufficient experimental investigations of multiphase flows, operational difficulties in handling biomass and the difficulty of controlling the fuel distribution between burners … as problems without available solutions" [4].

Understanding such flows and modeling them in detail would lead to greatly improved designs of multiphase flow reactors. This expectation is motivated by the numerous examples of successful application of single-phase CFD models that occurred during the last two decades. Single-phase CFD analysis is now routinely used in the aerospace and automobile industries and increasingly being used by the chemical and power industry. A chemical and engineered materials company concluded that, over a six-year period, the benefits accrued from the use of CFD resulted in a six-fold return on the total investment (including salaries) required in CFD [5]. Bish [6] gives the example of Hydro-Quebec where a CFD study of the hydroturbine helped to raise the turbine efficiency by 1.6% and resulted in estimated revenue gains of about $3.2 million per year. Hules and Yilmaz [7] describe how CFD has been used to analyze systems such as pulverizers, classifiers, ESPs, and SCR as well as utility furnaces and industrial boilers at Riley Power Inc. CFD modeling of burners "… saved many thousands of dollars of burner testing while cutting development time to a few weeks" and CFD modeling of air heaters "… pointed to places for simple and inexpensive



MFIX simulation of pilot scale KBR/Southern transport gasifier. C. Guenther, NETL.

improvement that otherwise might be overlooked" [7].

Multiphase flows are much more difficult to analyze than single-phase flows primarily because "the phases assume a large number of complicated configurations" [8]. Multiphase CFD modeling has been recognized as a tool with much potential, although it has not yet been developed to be used by itself for scale up [3]. The importance of multiphase CFD is also underscored by the fact that the Chemical-Industry-of-the-Future Technology Roadmap for CFD, written by representatives from the industry, identifies modeling dilute to dense multiphase flows as one of the highest priority items [9].

To get a sense of the magnitude of the challenges faced by the fossil fuel industry, we will use clean coal technology as an example. This technology is nationally important because of the abundance of coal in the United States and is a significant component of NETL's technology portfolio. To meet the demand for power in the United States, projections call for the construction of 87 GW of new coal-based power plants in the next 20 years [10]. That corresponds to 174 new 500-MW power plants, which requires an investment of over $100 billion [11]. The new plants will deliver power worth over $250 billion in the next 20 years[1]. The clean coal technology roadmap has set aggressive targets for efficiency, plant availability, capital cost, and cost of electricity (see Table 0.1) [12]. Furthermore the targets must be achieved with near-zero emission of pollutants including CO_2. And multiphase flow systems such as gasifiers form the centerpiece of clean coal technology. (See Appendix B for an example of the use of multiphase CFD models to help with the design of commercial-scale gasifiers). Therefore, the opportunity to address the multiphase flow challenges in fossil fuel industry is indeed a large one. Addressing those challenges themselves would lead to great economic benefits. The above example considers only new power generation in the United States. The opportunities are enormous when innovations in existing plants and power generation for the entire world are considered.

The challenges and opportunities in the fossil fuel industry presented in the last paragraph, although quite impressive, are small compared to those in the chemical, petrochemical, pharmaceutical, and consumer products industries. An estimated 40%, or $61 billion per year, of the value added by the U.S. chemical industry is related to particle technology [13]. A well-known Rand study has documented a distressing drop in plant performance when solids processing steps are involved. The average design capacity of solids processing plants is 64% compared to

1 Assuming a linear increase in the generation and Cost of Electricity (COE) = $35/MWh

90-95% for gas/liquid processing plants; start-up of such plants is delayed by approximately two years [14]. Although the Rand study is somewhat dated, there is no evidence that the problems reported in that study have been solved in a comprehensive manner. In fact, new problems have been added to the list. For example, exploration and colonization of the Moon and Mars may require that in-situ resources be processed for producing fuel or oxygen or both. "This requires us to understand the properties and mechanics of the extraterrestrial regoliths, to predict the behaviors of granular geomaterials in lunar and Martian environments, and to design technology capable of reliably controlling the various complex fluid flow regimes of these materials" [15].

Table 0.1. Clean Coal Technology Roadmap Performance Targets [12]

Performance Measure	Reference Plant	**2020 Plant**
Efficiency (HHV)	40%	**50-60%**
Availability	>80%	**≥90%**
Capital Cost, $/kW	1000 – 1300	**800 – 900**
COE, $/MWh	35	**<30**

Reference plant is one that can be built using current state-of-the-art technology and meets New Source Performance Standards.

Considering the national importance of multiphase flows, there have been efforts in the past to address the problems collaboratively. In 1995, a workshop on reactive multiphase flow simulation was held at Los Alamos National Lab "to start a dialog between Los Alamos and industry … for the initiation of a coordinated effort on substantially increasing the state-of-the-art of multiphase computational fluid dynamics" [16]. A Multiphase Fluid Dynamics Research Consortium (MFDRC) was established to advance multiphase CFD beyond the state-of-the-art achievable by any single business or laboratory through a partnership between three DOE National Laboratories, five petrochemical companies, an energy equipment manufacturer, and a computer manufacturer [17]. In 2002, a workshop on scientific issues in multiphase flow was held at the University of Illinois, which was attended by multiphase flow researchers primarily from academia. A general recommendation was made that "the emphasis of research in this area should change from a strictly engineering viewpoint (which has had limited success in developing general approaches) to a science-oriented one" [8].

In contrast to the previous workshops, the current workshop was focused on the application of computational multiphase flow to fossil energy problems. The workshop vision was *to ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants.* To achieve this vision, it is necessary to have focused and collaborative research in computations, theory, and experiments.

It is now widely recognized that computational science will play an important role in solving scientific and technological problems of 21st century. In fact, there is the great expectation that by year 2020 computational science will revolutionize the practice of science. The first great scientific breakthrough of this century – completing the decoding of the human genome in 2001 – is already a triumph of computational science [18]. A presidential advisory committee report states that "computational science now constitutes the *third pillar* of scientific inquiry, enabling researchers to build and test models of complex phenomena" [18]. Even that notion (of a *third pillar)* has been called "intermediate, unsustainable and undesirable" by a group of internationally recognized scientists; they make the stronger proposition that "… a leap from the application of computing to support scientists to 'do' science … to the integration of computer science concepts, tools and theorems into the very fabric of science" would occur by year 2020 [19]. Their report later states that optimized co-firing with biomaterials in coal-fired power plants would introduce new design challenges that would require "an improvement in complexity, resolution and visualisation of the flow, combustion and energy processes amounting to several orders of magnitude over" [19] the current models. In 1995 DOE's National Nuclear Security Agency (DOE-NNSA) launched the Accelerated Strategic Computing Initiative (ASCI) to ensure the safety and reliability of the nation's nuclear stockpile through computer simulations rather than testing [20]. In 2001 DOE's Office of science (DOE-SC) established the Scientific Discovery through Advanced Computing (SciDAC) program boldly affirming "the importance of computational simulation for new scientific discovery, not just for 'rationalizing' the results of experiments" [21].

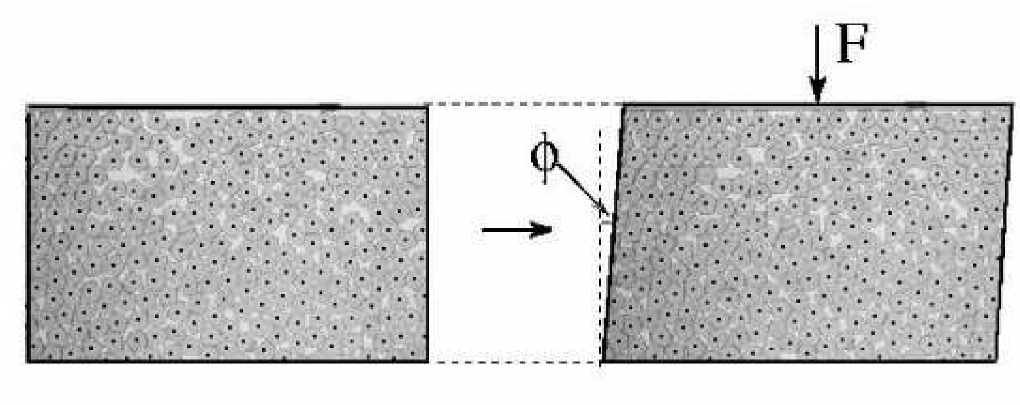
There are several common issues that need to be addressed for the large-scale application of computational science. They are relevant to the discussion in this report as well: collection, storage, and analysis of large volumes of scientific data [19, 20]; the recognition that computational science work would be “predominantly multidisciplinary, multi-agency, multisector, and collaborative” [18]; the need for making the simulation tools science-based and, thereby, improving their predictive capability [19, 23]; and the need for detailed verification and validation of the simulation tools [23, 24].

The workshop discussions were held under four technical tracks: (1) Dense gas-solids flows and granular flows, (2) Dilute gas-solids flows, (3) Liquid-solids and gas-liquid flows, and (4) Computational physics and applications. The planning for each track was done by a track chair from industry, a co-chair from a university, and an NETL champion. The track chairs initiated a web-based technical discussion prior to the meeting. They presented a summary of the findings in four technical track presentations on the first day (see the agenda in Appendix A). The topics were then discussed in four parallel technical track breakout sessions, which were moderated by the track chairs. On the second day, the track chairs presented a summary of the previous day’s discussions. This was followed by a presentation on the integration of the tracks and a general group discussion.

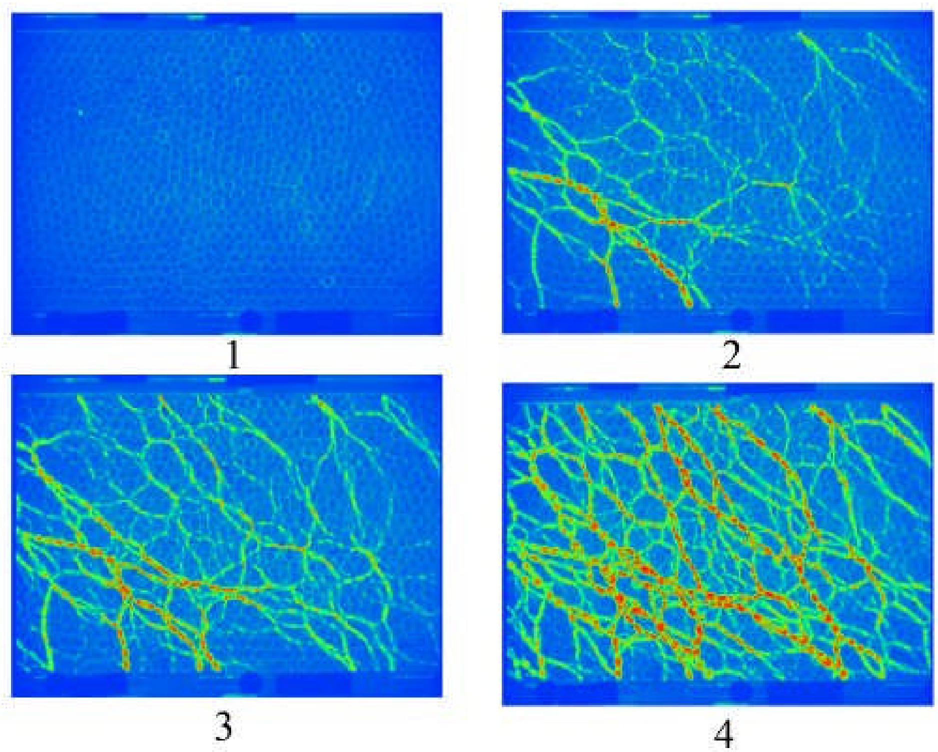
The track chairs wrote track reports based on information discussed at the meeting and information collected from researchers who could not attend the meeting. All the workshop participants were given the opportunity to review and comment on the report before it was released. A compilation of the track reports and other supporting information resulted in this report. Experts in the field, whose names are shown at the end of each section, wrote the different sections. The information from the track reports were condensed, compiled, and categorized to develop the technology roadmap given at the end of this report.

The main outcome of the workshop is this report outlining the research needs in multiphase flow. It is hoped that the workshop will improve the visibility of multiphase flow research, help influence future research solicitations, and spur collaborative research. A collaborative effort is already underway in the form of a Collaboratory for Multiphase Flow Research (CMFR) being formed by NETL, Carnegie Mellon University, the University of Pittsburgh, and West Virginia University. Further collaboration among researchers from industry, academia, and national labs from across the nation will allow the increasingly limited R&D investments to be used more effectively to solve critical multiphase flow problems of national importance.

♦ M. *Syamlal*



(a)



(b)

Stress chains in shearing dense granular media: In granular materials, force is rarely transmitted uniformly, but rather preferentially along a network forming force chains. The above photos show experimental demonstration of force chains obtained using shearing photoelastic disks. Note that some of the disks in the photo are not colored at all (no force), while the disk right next to it is highlighted in the color red (high force). R.P. Behringer, Duke University.

1 Dense gas-solids flows and granular flows

The objective of this track is to identify the key research questions that need to be addressed in order to advance the state of knowledge and modeling capability for dense particulate flows, especially as applicable to energy applications. Most of these questions were pre-identified going into the workshop, drawing on the report of the IFPRI Working Group on Powder Flow [18]. During the workshop, the Track 1 participants amended this list and then grouped the individual items into four topical groups (Tables 1.1-1.4), with the intention that these groups can provide a more efficient research strategy within the NETL Collaboratory. These groups were then prioritized according to a proposed timeline (Figure 1.1).

Table 1.1: Fundamental aspects of stress and flow fields in dense particulate systems.

- What defines the stress and flow fields for the relevant flow regimes?
- How is stress transmitted throughout the material?
- How are these related to boundary conditions, particle properties, and process control parameters?
- What sets the stress and flow fields for the relevant flow regimes?
- How are stress changes or changes in other quantities transmitted throughout the sample?
- What is the character of fluctuations that occur in stresses/forces and flow fields?
- What parameters control the transitions between different granular states, e.g. quasi-static vs. intermediate? What is the nature of these transitions?
- What is the range of states that is compatible with a given set of (boundary) control parameters? The answer to these will address the repeatability issue.

Table 1.2: Definition of material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements.

- How should one characterize a granular mixture, particularly one where the particles have a continuous range of sizes, shapes, and/or surface properties?
- Given that real granular materials may require a very large number of parameters for a complete physical description, what are the most useful truncations of such a parameter space that give reasonably accurate characterization?
- Need to define key material parameters (interparticle forces…)
- What experimental (and simulation) methods are most useful in a) addressing basic physical questions, and b) providing key insights for practical applications?
- What diagnostics can be used to infer information of flow fields and stresses both internally and at the boundaries? Develop criteria to expose when the interstitial fluid flow is important in a given problem involving powder flow.
- Develop quantitative models for the effects of vibration and pressure pulsations generated through a microphone – either by themselves or in conjunction with fluidizing gas flow – on the dynamics of particle agglomerates.
- For publications, encourage reporting of experimental and simulation conditions, environmental, boundary conditions, material properties, etc.
- Develop a cumulative table of metadata
- Identify and connect with appropriate standards organizations (NIST, ASTM, ISO, etc…).
- Collaboratory round robin or grand challenge addressing both experimental and simulation (DEM, continuum, constitutive) components.

Table 1.3: Given the practical need for continuum modeling capability, identify the inherent limitations and how to proceed forward, e.g., hybrid models that connect with finer scale models (DNS, DEM, finite element, stochastic, etc.) for finer resolution.

- How to define continuum strategy?
- How to define continuum and high-resolution criteria in a hybrid model, e.g., based on structural inhomogeneities and/or discontinuities?

- What mathematical approach can be used to incorporate flow and stress fluctuations into a suitable theory (e.g., Langevin approach for random uncorrelated fluctuations, extended granular temperature…).
- Is there a connection between the possible states consistent with control/boundary conditions, and the range of fluctuations seen? What is the nature of repeatability tied to fluctuations?
- Develop a physical understanding of the effect of interparticle forces on the hierarchy of flow-induced inhomogeneous structures.
- Develop a better understanding of stick-slip motion of cohesive powders and how it can be manipulated to get optimum flow and mixing characteristics
- Probe the effect of microstructure on the drag coefficient.
- Develop continuum rheological models for assemblies of particles (2 and 3 phase) – from quasi-static to rapid flow regimes, bringing in the path- and history- dependence (compression, dilation) manifested by cohesive systems. Use experiments, simulations, statistical frameworks.

Table 1.4: Size-scaling and process control (particle / unit-op / processing system) is critical to industrial applications.

- How are stress and flow fields in a unit operation related to boundary conditions, particle properties, and process control parameters?
- What is the response of a system to a change at the boundaries?
- In a dynamical process, what is the relation between energy input (power) and flow?
- System integration – how to connect models to control and/or optimize an integrated system (e.g,., multi-variate PBM's…)
- How to apply available scale-up and process control knowledge to energy-based systems, including:
    - Fluidization
    - Coal gasification, predict carbon utilization as a function of operating conditions
    - Dry feeding into high T, P environments; a-priori simulation followed by (costly) experimental validation

1. Fundamental aspects of stress and flow fields in dense particulate systems.
2. Definition of material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements.
3. Given the practical need for continuum modeling capability, identify the inherent limitations and how to proceed forward, e.g., hybrid models that connect with finer scale models (DNS, DEM, finite element, stochastic, etc.) for finer resolution.
4. Size-scaling and process control (particle / unit-op / processing system) is critical to industrial applications.

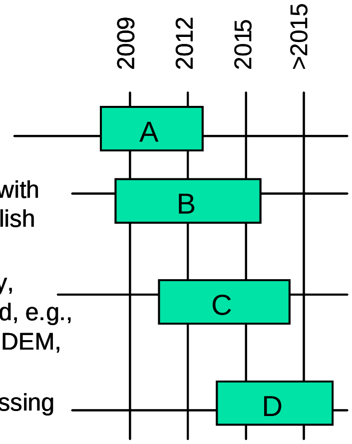
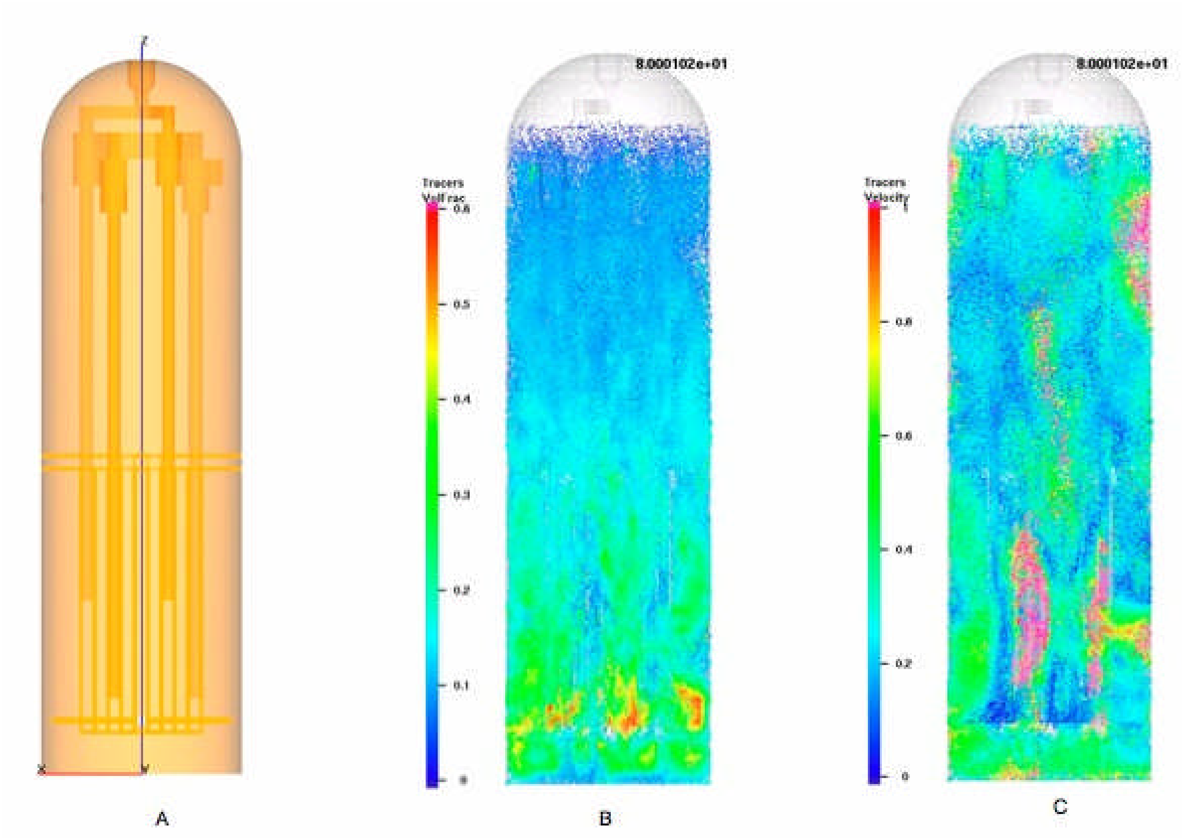


Figure 1.1. Strategic timeline for addressing key topical areas related to dense phase flows. Block A is primarily concerned with the issues in Table 1.1; B refers to issues in Table 1.2; C refers to Table 1.3 and D refers to Table 1.4..

♦ *Paul Mort and Joseph McCarthy*



Three-dimensional simulation of an industrial-scale (4.6 m diameter) turbulent dense-bed reactor with complex internals: 6 cyclones, spargers, cooling coils. Gas superficial velocity is 0.7 m/s and discrete particle sizes range from 20 to 280 microns at a density of 1950 kg/m^3. Results at 80 seconds: A – reactor geometry; B – solids concentration showing the effects of dipleg feeds and spargers; C – solids velocity showing gas bypassing. Simulations performed with Barracuda CPFD® commercial software. K. Williams, CPFD Software, LLC .

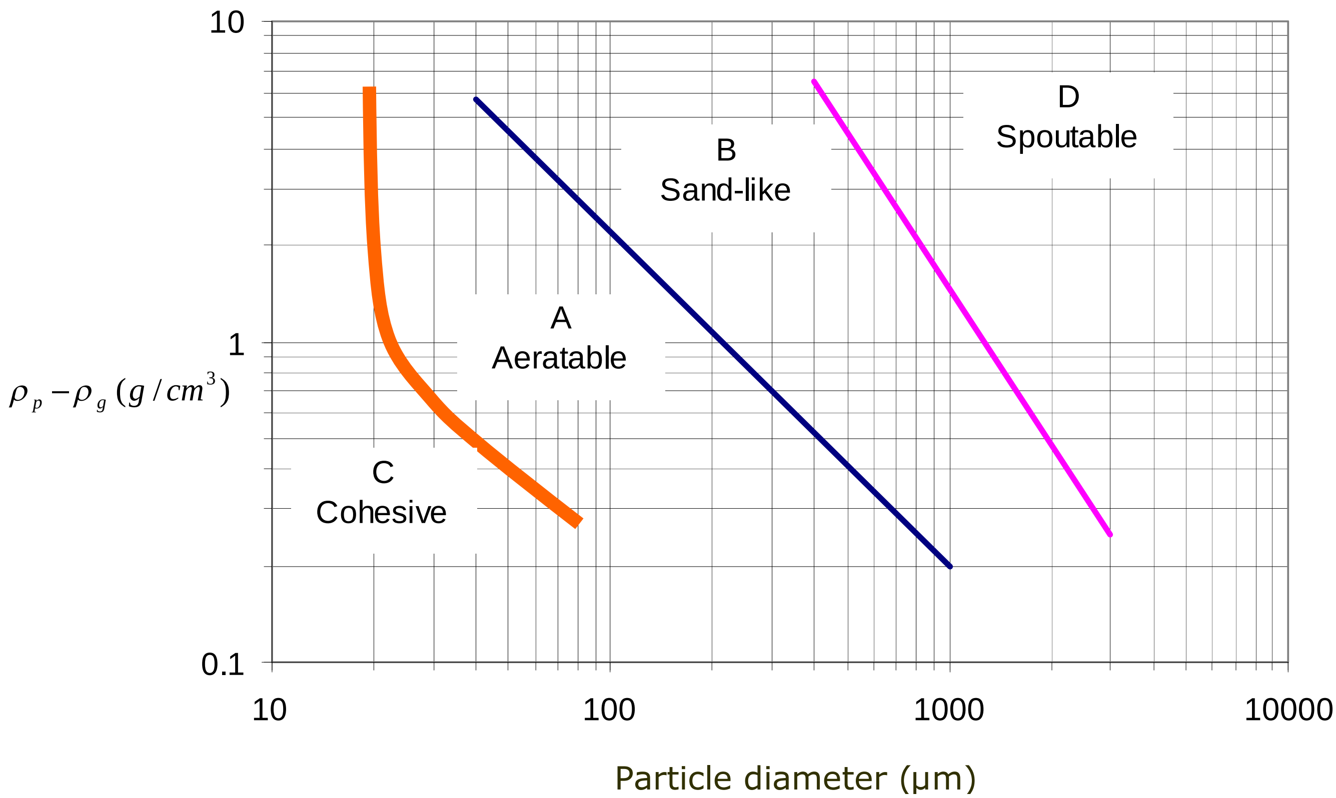


Diagram for classifying powders into groups having broadly similar fluidization characteristics in air at atmospheric temperature and pressure [121].

2 Dilute gas-solids flows

Introduction

Flows involving solid particles in contact with a carrier gas are ubiquitous in nature and industry. Industrial applications range from fossil fuel processes—such as fluidized bed combustion, fluid catalytic cracking (FCC), and coal gasification—to manufacture of chemicals, petrochemicals, and pharmaceuticals. The scope of this track encompasses gas-solids flows with average solids loadings up to about 5 vol%. In practical applications this range of solids concentrations is present in a variety of situations -- riser reactors, combustors, dilute conveying, etc. In these applications, while average concentrations are lower than 5 vol%, there are almost always regions with much higher solids concentrations up to close packing. For example, in riser reactors or coal combustors, the riser section which is relatively dilute is preceded upstream by a region that is much denser – the entrance region of the reactor. Further, even in the developed region of a riser, the annular zone has much higher concentrations of solids than the core or the average. It follows that there is an overlap between dilute and dense flows, and development of dilute gas-solids models must include consideration of denser regions and the transition from dense to dilute.

State-of-Art Summary

Typical industrial devices in which these flows are encountered are notoriously hard to design and scale up [3]. While multiphase computational fluid dynamic modeling has been recognized as a tool that has much potential in process design [3], there is an urgent need for improvements in multiphase CFD [26]. The Chemical Industry of the Future's Technology Roadmap For Computational Fluid Dynamics identifies modeling dilute-to-dense multiphase flows as one of the highest priority items [9].

Multiscale characteristics: One of the principal difficulties in multiphase CFD modeling is the multiscale nature of the problem [27, 28], i.e., the difficulty in bridging the wide range of length and time scales over which physical phenomena manifest themselves, and the interaction between these scales. Broadly speaking, three ranges of scales are recognized: microscale phenomena observed at the scale of the particles themselves, mesoscale phenomena observed on the order of 10-100 particle diameters, and macroscale phenomena observed on the scale of the industrial device (see Fig. 2.1).

Particle Clustering: A typical multiscale phenomenon that poses a challenge to CFD modelers of multiphase flow is the clustering of particles that occurs in gas-solids suspensions in the range of volume fraction from a few percent to about 30%. This phenomenon manifests itself at the macroscale in circulating fluidized bed risers and is observed as a markedly inhomogeneous solid particle volume fraction profile in the radial direction consisting of two characteristic regions: a dilute gas-solid suspension preferentially traveling upward in the center (core) and a dense phase of particle clusters, or strands, that can move downwards along the wall (annulus) (e.g. [29, 30, 31]). Depending on gas velocity, the annular region can also move entirely upwards. These clusters and streamers of particles, whose characteristic size is on the order of 10-100 particle diameters [32, 33], are termed mesoscale structures and they significantly affect the overall flow behavior. Experiments conclusively reveal that particles do form clusters [34, 35, 36], and these clusters significantly affect the macroscopic flow characteristics. A variety of mechanisms may induce particle clustering including the dissipative nature of interparticle collisions, turbulence, and hydrodynamic interactions with particles resulting in enhanced local energy dissipation in the fluid. In addition, van der Waals attractive forces can dominate interactions among Geldart C cohesive particles [37].

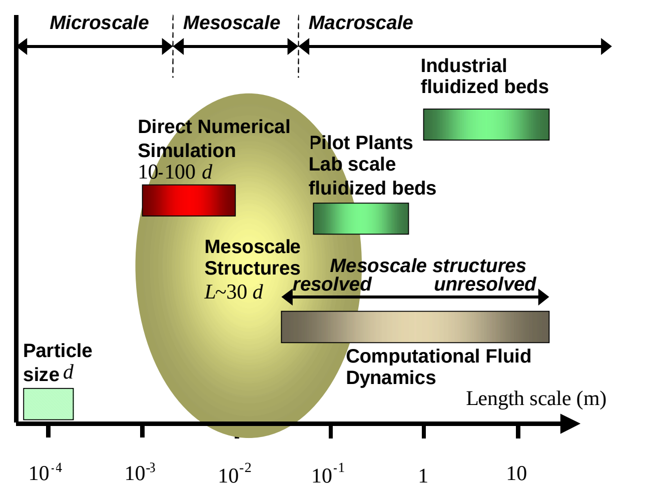


Figure 2.1. Length scales in CFB risers.

Particle-particle collisions can be significant even in dilute flows as noted by Hanratty et al. [38]. The dissipation of energy due to inter-particle collisions is the main mechanism for the formation of clusters as demonstrated by the simulation results of Tanaka et al. [39]. In fact, Figure 2.2 shows clusters forming at dilute conditions for an average solids volume fraction of 10^{-4}. Other experimental and simulation studies have shown the existence of clusters at low solids volume fractions as demonstrated by Ito et al. [40].

Macroscale picture: For the dilute to moderately dense gas/solids flows considered in Track 2, several approaches are being used to model these flows: The continuum approach (also called Eulerian or two-fluid model) is the method of choice for simulating industrial-scale systems. Most of the different approaches used currently are summarized by van Wachem et al. [41], Enwald et al. [42] and Gidaspow et al. [43].

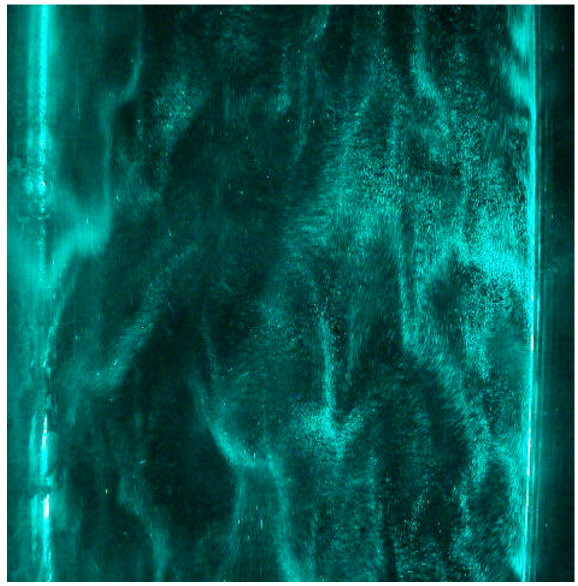


Figure 2.2. Cluster structures from experiments of Tanaka et al. (2002).

Discrete approaches, such as discrete particle method (DPM) or Lagrangian Eulerian (LE) methods, which do not take into account particle-particle collisions, are not useful to model dilute to moderately dense flows because collisions are important even at very low solids volume fractions (10^{-4}) as noted by Hanratty et al. [38]. Other discrete methods that take into account particle-particle collisions are used to study particulate systems. These techniques include soft-sphere model, or DEM [44, 45] and the hard-sphere model used by Galvin et al. [46] to verify/validate continuum kinetic theories. Ye et al. [47] have used hard-sphere simulation data to estimate parameters used in the soft- sphere model as well as propose a cohesion model for the continuum approach.

CFD calculations of fluidized beds solve averaged conservation equations in each phase [48, 49, 50]. Closure of these equations requires modeling of average stresses [51, 52, 53] and second moments of the fluctuating velocity in both phases. Jackson's book [37] describes the evolution of riser flow calculations [54-59] starting from one-dimensional flow in a vertical pipe [60] to current state-of-the-art CFD calculations [53, 61]. The importance of fluctuations in the particle velocity has been established [35, 59], and the effects of gas-phase turbulence have also been examined [58, 62, 63, 64] to a somewhat lesser degree. Phenomenological models of cluster drag have been proposed to explicitly account for the formation of clusters [34, 65-67], but these have shown limited predictive capability. While current CFD codes are capable of reproducing the core-annulus flow in risers [54, 56, 57, 63], persistent difficulties are sensitivity to models and model constants, and numerical convergence issues. Sundaresan and co-workers showed that CFD calculations of fluidized beds do not have sufficient resolution to capture inhomogeneities in the mean volume fraction that appear at the mesoscale [53]. This has motivated coarse-graining approaches to bridge the mesoscale to the macroscale, and thus explicitly account for this under-resolution [61]. Recently, Jiradilok et al. [118], compared kinetic theory based CFD simulations to various experiments.

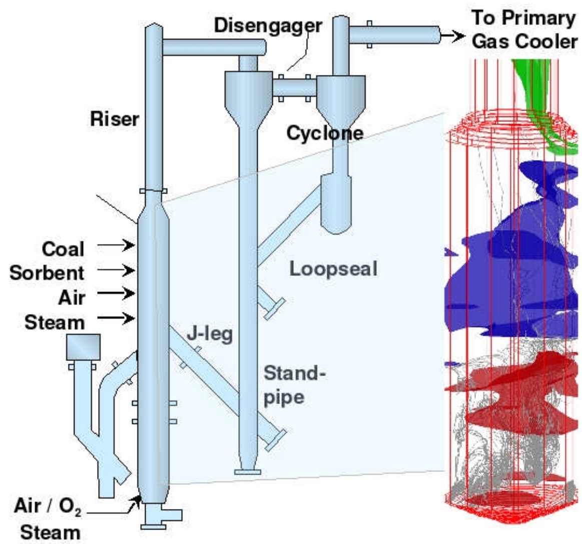


Figure 2.3. Results from an MFIX simulation of the PSDF gasifier for the mixing zone (identified in the schematic on the left), shows the oxygen concentration superimposed on isosurfaces of at void fraction values of 0.9. [69]. Source: www.mfix.org

Typical CFD calculations use empirical correlations for heat and mass transfer in gas-solids flow [68]. One of the difficulties in CFD modeling of risers (see Figure 2.3) is accounting for chemical reactions. The large number of chemical species and reactions results in significant computational overhead that adds to an already challenging hydrodynamics problem. This precludes the incorporation of detailed chemical kinetics, and reduced reaction mechanisms or simplified kinetics are typical. In this context, recent advances in automated simplified chemical mechanisms (Intrinsic Low-Dimensional Manifold, ILDM [70], Computer Singular Perturbation, CSP [71]) or on-the-fly tabulation schemes for reaction rates (ISAT [72]) are very promising. Of the two approaches, although the automated reduction approaches are mathematically elegant, it is the tabulation approach that has enjoyed more success in practical applications [73].

Mesoscale picture: The stability of homogeneous suspensions has been extensively studied using averaged equations (continuum models) of gas-solid flow as a starting point. Glasser et al. [74, 75, 76] have shown that the averaged conservation equations of gas-solids flow admit traveling wave solutions that represent instabilities, and these instabilities result in inhomogeneous volume fraction fields that correspond to clustering in dilute suspensions. These instabilities arise due to an interaction between particle inertia, gravity, and gas-particle drag, and the characteristic length scale of these structures is given by $L = (\mu_s v_t / \rho_s g)^{1/2}$ [53] (here v_t is the terminal velocity of the particle, and μ_s and ρ_s are the dynamic viscosity of the solid phase and density of a single particle, respectively). However, the phenomenological nature of the closures inherent in the averaged equation approach, and the models for quantities like μ_s, precludes a first-principles explanation of clustering at the mesoscale in terms of microscale interactions.

Microscale picture: Koch [77] has developed a kinetic theory for dilute monodisperse gas-solid suspensions in the limit of low Reynolds number and high Stokes number $St = \rho_s d T^{1/2} / 9\mu_f$ (here the Stokes number is based on the particle fluctuating velocity which scales as square root of the granular temperature, *T*; d is particle diameter and μ_f is fluid viscosity (See Figure 2.4). This theory is applicable to suspensions where particle inertia is predominant (elastic collisions are accounted for) and fluid interactions are accounted for but are purely viscous (fluid inertia is not important). The analysis exploits the fact that hydrodynamic interactions in this limit are long-range, whereas collisional effects are short-range. Stability analysis of the averaged equations indicates that the suspension is unstable to particle density waves, with particle inertia providing the destabilizing mechanism while the energy lost by particle fluctuating motions to viscous flow interactions is stabilizing. For this limiting case, Koch's microscale analysis shows that the flow of particle suspensions in the regimes of low-to-intermediate levels of particle volume fraction ($\phi^{-3/2} << St$) does not remain homogeneous, but exhibits instabilities and structures. This theory has been extended to higher volume fraction by Sangani et al. [78]. While this theoretical work lays the foundation for microscale study of suspensions, it is limited in applicability to fluidized beds because it

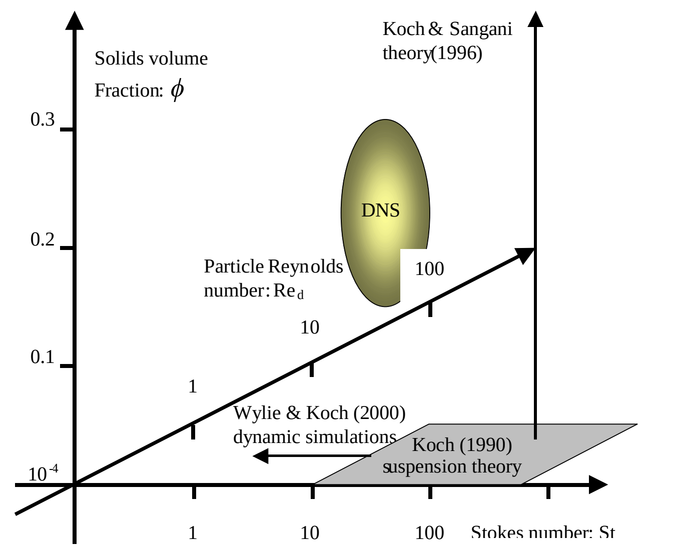


Figure 2.4. Suspension microscale regimes showing limits of theory and simulations.

neglects fluid inertia, which is important at the particle scale in riser flows. Also it has been pointed out that neglecting the gas phase oscillations causes the predicted granular temperature to be much smaller than experimental data [79].

In a recent review article on inertial effects in suspensions [80], Koch notes that suspensions with significant microscale fluid inertia, which will typically be turbulent, pose significant challenges to theoreticians due to nonlinearity, unsteadiness, and short-range hydrodynamic interactions. Direct numerical simulation of suspension flow [81-85] is a powerful tool to analyze these flows. Wylie and Koch [86] show through dynamic simulations of an isotropic suspension of elastic colliding particles in a viscous gas, that as the suspension loses energy the particles tend to cluster as indicated by more near neighbors than in a hard-sphere distribution. This study also established the limits of applicability of the high Stokes number theory [78], and showed significant deviations from the theory for $1 < St < 10$.

Direct Numerical Simulations: Several approaches have now been developed for solving the Navier-Stokes equations governing flow over fixed and moving particles at finite Reynolds number with exact boundary conditions imposed on each particle surface [87-97]. Only recently have these simulations accounted for turbulence [98], although a large number of numerical studies [99-104] have been performed on turbulent particle-laden flows assuming point particles (those studies are not relevant to suspensions because they assume the particles are much smaller than the Kolmogorov scale of turbulence, and they neglect shielding or blocking effects on neighbor particles because the flows are very dilute).

From this brief and topical review of current work on particle clustering, which is far from comprehensive, it is clear that our understanding of the mechanism(s) underlying cluster formation and the generation of volume fraction inhomogeneity is still far from complete for suspensions with microscale particle inertia and moderate Stokes number.

Workshop Outcome

The ultimate goal or vision from the workshop is a CFD code that is capable of modeling a gas-solids flow reactor, for example a coal combustor or a FCC reactor, thus requiring coupled solution of hydrodynamics, heat and mass transfer, and chemical reactions in both gas and solids phases. In some cases, FCC being an example, a liquid feed is also present which evaporates and reacts and is converted in the reactor to mostly vapor products. Naturally, such a code needs to run and converge in a reasonable amount of time to be useful. While we are far from the ultimate goal, even today industry uses CFD to model such reactors using a certain amount of empiricism to overcome limitations in the models. The roadmap for code development is a methodical path to gradually and systematically introduce improvements in the models to reduce the level and extent of empiricism and rely instead on fundamentally based models. During this journey, we envision continued application of multiphase CFD to modeling such reactors so that we take advantage of improvements as they are developed, meaning that practical applications must be kept in mind during model development.

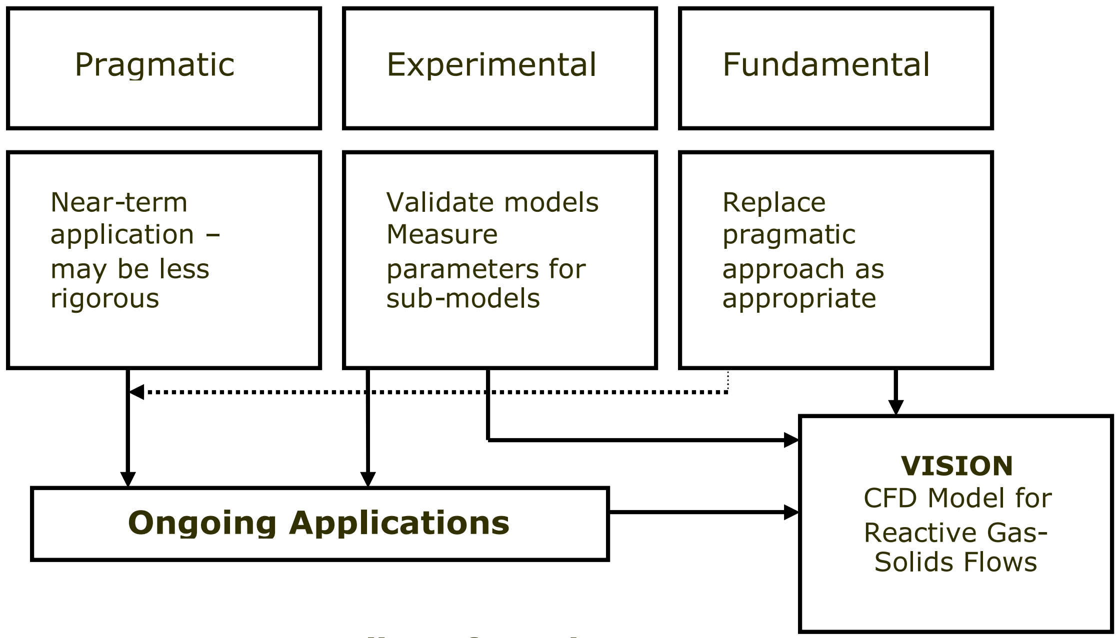
Discussions prior to and during the workshop developed the roadmap under three themes:

- Pragmatic: Modeling improvements that could be applied in the short term for more accurate predictions for practical problems. These would emphasize utilitarian shorter-term solutions which might be more empirical.
- Experimental: Specific experiments needed to validate models and measure key parameters
- Fundamental: Modeling improvements directed at fundamental phenomena that are inadequately addressed in current models and that could reduce or eliminate empirical assumptions. Most but not all of these would become useful in the longer term.

We envision that the thrusts under the above themes would be progressed essentially in parallel. Industry could take advantage of pragmatic improvements yielding benefits in the short term; fundamental advances would be incorporated into models, gradually finding their way into models in practical use; and experimental data and measurements would ensure that the models represent reality. Progress along these lines will maintain industrial interest, which is crucial in sustaining development of industrially useful models, and creating a healthy environment for model development.

Recommendations

Recommendations from the workshop are divided into near-term, mid-term and long-term time frames. Under each time frame, we have listed the recommendations under three themes: pragmatic, experimental, and fundamental. Finally each recommendation has been given a priority: High (**H**), Medium (**M**), or Low (**L**). Some recommendations spanning two priorities—Low-Medium (**L-M**) and Medium-High (**M-H**)—are also indicated



Outline of Roadmap

Near Term (1 – 5 years)

Pragmatic

1. Develop a drag law applicable over the entire range of solids fraction. Current drag laws do not give correct results in CFD models over the range of solids concentration encountered in practical problems. The drag law needs to account for fluid-particle forces at particle scale including the effect of neighbor particles. Such an improved drag law would find immediate application in existing CFD codes. **H**
2. Develop efficient methods for industrial scale computations emphasizing treatment of relatively large size cells. Continue development of coarse graining (filtering) of two-fluid models. See Fig. 2.5. This approach allows more accurate simulation of gas-solids flows in industrial applications where the scale of equipment demands use of relatively coarse meshes for reasonable execution times. Evaluate other approaches as they are developed. **H**
3. Develop models and constitutive relations to handle particle size distributions. This could involve developing a computational framework with speedy computation, validated constitutive models, and multi-particle kinetic theories. A subset of this effort would

involve two-fluid or E-E models for particle deposition and re-suspension accounting for particle size distribution effects [e.g., 105, 106]. **H**

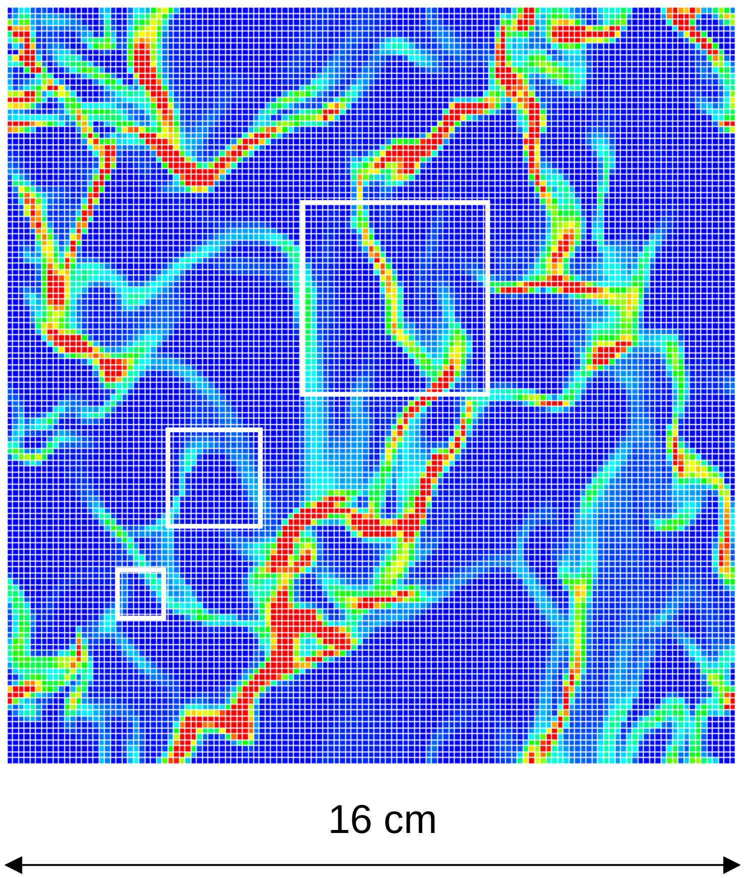


Figure 2.5. Snapshot of particle volume fraction fields obtained while solving a kinetic theory based two-fluid model. Fluid catalytic particles in air. 128 x 128 cells are shown in the figure. The average particle volume fraction in the domain is 0.05. Red color indicates regions of high particle volume fractions. Squares of different sizes illustrate regions (i.e. filters) of different sizes over which averaging over the cells is performed. From A. T. Andrews IV & S. Sundaresan, 2005 AICHE Annual Meeting, Paper 209a, Cincinnati, Nov 1, 2005

4. Develop reduced order models from accurate computational results for use by design engineers. **H**
5. Develop models for non-spherical particles. **M**
6. Account for particle-particle collision and its effects on momentum and angular momentum transfer, along with heat and mass transfer. **L**

Experimental

1. Build and operate gas-solids flow facilities to provide high quality detailed data for at least two scales: ~ 0.15 m and ~ 0.6 m diameter. The facility would include well-characterized entrance and exit conditions for gas and solids including pre-conditioning of the gas-solids inlet flow, along with well-characterized boundaries. Detailed measurements should be taken of characteristic local variables such as velocity of gas and solids, solids fraction, solids flux, fluctuating quantities, cluster size, etc., using advanced instrumentation without excessive intrusion that would disturb the flows. The data from the facility would be used to test and validate models. Two length scales are needed to capture the effect of scale on flow characteristics and to increase confidence in model predictions for industrial scale simulations. We envision a multi-year program in this facility to obtain the required data. Although it will involve significant costs, consideration should be given to allow operation at temperatures and pressures above ambient because most industrial processes involve such conditions. **H**
2. Calibrated, non-intrusive diagnostics need to be used to make measurements in the flow facility. Various techniques are available today but improvements are needed to overcome present limitations. In general, there is need for simultaneous measurements in the gas and solids phases, and measurement of planar flow fields rather than point-to-point traverses. Measurements should include turbulent fluctuations. Full-field visualizations of translational as well as rotational motions of spherical and non-spherical particles (2-D and 3-D geometries and measurements) are needed to understand and model frictional interactions among particles. **H**
3. While the large flow facility is needed to provide data in geometries akin to industrial processes, there is also a pressing need for very specific small-scale experiments to provide data to improve and check sub-models. As an example, cleverly designed experiments are needed to measure simultaneously drag in gas-solids flows as well as gas and solid velocities (slip). **M**
4. Another important area is the effect of walls on flow. Near-wall measurements using sophisticated techniques are needed to establish wall boundary conditions for the models. **M**

Fundamental

1. Address correct procedures for boundaries. Exits – how to handle solids versus gas boundary conditions. Walls – do simple conditions (e.g., no slip) capture physics? Use DEM or other techniques to resolve. **H**

2. Particle Clustering. An understanding of the basic physics of clustering is needed. The instability mechanisms leading to fluctuations in concentration, and the scaling of the competing physical mechanisms with nondimensional parameters is required. These need to be integrated into a predictive model for particle clustering. The effect of particle clustering on drag, collisions, and gas-phase turbulence modulation also need to be modeled accurately. **H**
3. Development of kinetic theory for continuum models based on qualitative and quantitative input from discrete models, which are based on fewer assumptions than the continuum approach. For this purpose, the hard-sphere model can be used to verify/validate continuum kinetic theories as demonstrated by Galvin et al. [46]. Also, Ye et al. [47] have used hard- sphere simulation data to estimate parameters used in the soft- sphere model and proposed a cohesion model for the continuum approach. **M-H**

Mid Term (5 – 10 years)

Pragmatic

1. Develop initial fully coupled reactive flow model. **H**
2. Develop automated procedure to coarsen hydrodynamic non-reactive or simple reaction results from CFD for use with more complex reaction networks. This approach would allow relatively rapid CFD calculations (no or simple reactions) giving detailed flow and pressure field. The coarsened results (effectively a network of CSTRs) coupled with more detailed reaction kinetics would give more rapid execution to predict yields. (This process is being used by some industries and perhaps others today but it tends to be ad hoc, labor intensive, and time consuming. The automated procedure would save time and be more reliable.) **H**
3. Develop pragmatic approach to handle particle attrition and agglomeration as they affect hydrodynamics and reactor performance. **L-M**

Experimental

1. Use large flow facility to elucidate the effect of particle size distribution on flow. Initial experiments with binary mixtures to determine lateral distribution of particle sizes and segregation. **M-H**
2. Continue experiments using continuous particle size distribution and measure spatial variation of particle size in flow field. **M-H**
3. Make measurements for characteristic parameters used in models such as collisional parameters, internal angle of friction, etc. **M-H**

4. Make detailed measurements in reactive gas-solids flow with simple chemical reaction, e.g., ozone decomposition. **M**
5. Devise simple experiments to determine importance of flow-generated electrostatic forces on dilute gas-solids flows for both cold and hot (process) conditions. **M-H**
6. Devise experiments to measure flow fields in the presence of obstacles, such as heat transfer tubes, baffles, etc. **M**

Fundamental

1. Develop in-situ adaptive tabulation of chemical reaction rates for heterogeneous reactions and couple with full CFD simulation for reactive flows. **M-H**
2. Modeling multiscale interactions. Develop models and codes that explicitly recognize and account for the micro/meso/macroscale picture that is emerging from studies at these different scales. **M-H**
3. Filtering procedures to rigorously extend LES to multiphase flows. The traditional LES approach relies on a separation of scales and a simple model for the small scales of turbulence. The core ideas of the LES approach can be profitably used in multiphase flows provided care is taken to account for the multiscale interactions and lack of scale separation. **M**
4. Theoretical challenges in mathematical formulations of multiphase flows. The steady RANS equations for single-phase turbulence obtained by omitting the unsteady term in the RANS equation set, admit numerical solutions. However, if the corresponding unsteady terms in the averaged two-fluid equations are omitted, the system does not always admit stable analytical or numerical solutions. It is common practice to time-average the unsteady solutions to the two-fluid equations and present those as the statistically steady solutions. This points to a deeper problem in the mathematical formulation of the two-fluid equations and needs to be addressed conclusively. **M**
5. Develop methods to account for particle dispersion in solid-fuel injectors and gasifiers. We need to simultaneously account for particle dispersion as well as fluctuating kinetic energy. **M**
6. Test models for prediction of temperature and pressure effects and for transition between Geldart A and B classifications using available data. **M**
7. Determine significance of gas emanation from particles (via chemical reactions) on overall hydrodynamics and develop models to handle if required. **M**
8. Develop methods to model adsorption/desorption and heterogeneous chemical reactions. **M-H**

9. Develop theory to model liquid feed injection and subsequent evaporation of liquids. (Needed for reactors with liquid feed.) Issues include: liquid-solid-vapor mechanics, capture of liquid by particles and vice-versa; transport of wetted solids and subsequent redistribution of liquid to other particles; different mechanics of liquid coated particles – stickiness, evaporation of liquid, and chemical reactions. **M**
10. Determine significance of electrostatic forces and van der Waals (cohesive) forces on hydrodynamics and model as appropriate. It is well known that significant static charge can be built up in cold-flow fluid-bed systems, and particularly in circulating fluid beds (CFB). Electrostatic shocks and strong sparking discharges have been reported by experimenters. These charges appear to be generated by collisions of particles with each other and with the walls of the units which are often non-conducting plexiglas. Interestingly, no such behavior is reported in commercial CFBs, such as FCC units, even though many of these are completely lined with non-conducting refractory. An exception is in gas phase polymerization reactors where charge measurement instruments indicate high static charge levels. There is thus a need to establish the importance of electrostatic forces on hydrodynamics and the dependence on conditions such as temperature, gas and solid properties, etc. For cohesive particles (Geldart C), there is a corresponding need to assess and model the effects of cohesive forces on hydrodynamics. (Mid-term Experimental recommendation 5 above complements this recommendation.) **M-H**
11. Test models for flow in the presence of obstacles such as heat transfer tubes, baffles, etc. **M**
12. Determine significance of radiative heat transfer (particle-particle and particle-wall) for high-temperature beds and model as appropriate. **L-M**
13. Develop model for erosion of walls/ internals by particle impact. **M**

Long Term (10 – 15 years)

In the long term, we expect that fundamental advances would have replaced pragmatic approaches and that sufficient data will have been obtained for sub-model development and code validation. At this stage, the following are recommended:

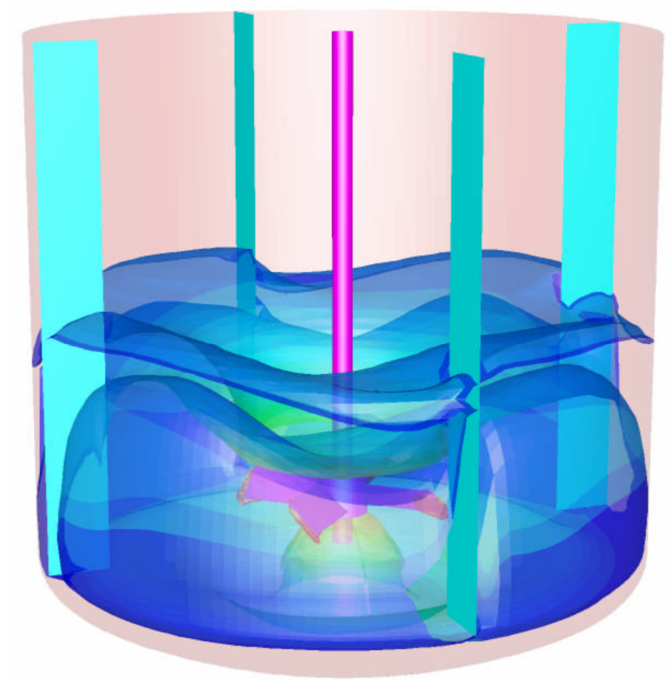
1. Integrate developments to complete fully coupled reactive flow model for industrial-scale reactors capable of handling a range of mesh sizes with reasonable run times.

♦ *R.D. Patel, S. Subramaniam, S. Benyahia*

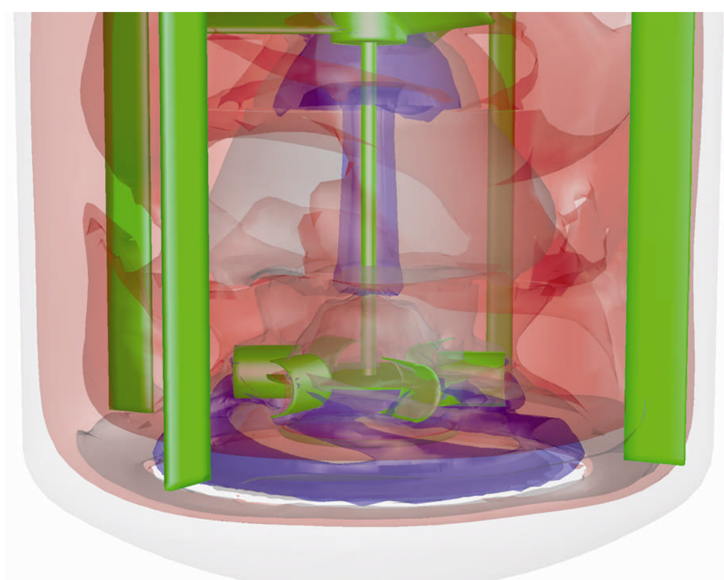
Present Day Pragmatic Modeling of Industrial Riser Type Flows

While dilute gas-solids flows are still insufficiently understood and CFD models far from complete today, it is still possible to obtain useful results from the models for practical situations in industry. As an example, current models and understanding have been used to successfully model flows in industrial risers. This is done using judicious approximations and simplifications and tuning model parameters using macroscopic cold flow and other data.
CFD modeling of industrial-scale risers necessarily means using computational meshes too large to capture particle-scale phenomena. As a result, straightforward application of CFD packages with such meshes with actual average particle size will inevitably give erroneous results. One pragmatic approach to resolve the problem is to use an average cluster size instead of the actual particle size. The cluster size is chosen to match experimental measurements in risers of different scales. This approach can be used to model industrial risers particularly in the developed core-annular flow region.

♦ *R.D. Patel*



Iso-surfaces of solids volume fraction in a stirred tank, simulated using the Eulerian granular multiphase model; the distribution of solids in the vessel was compared to experimental data using a variety of drag laws and one that incorporated the local turbulence field worked best. A. Haidari, Fluent Inc.



Surfaces of nitrogen gas, sparged into a two-impeller mixing tank; studies such as this are used to optimize the location, size, and speed of the impellers for the most uniform gas distribution, an important condition for mass transfer between phases. A. Haidari, Fluent Inc.

3 Liquid-solids and gas-liquid flows

The overall objectives for multiphase flow research for gas-liquid and liquid-solids systems (as shown Figure 3.1) are to be able to model the flow regimes and detailed phase distributions, to effectively and accurately predict heat and mass transfer across various flow regimes, and to use software codes for industrial scale-up and applications. To achieve these objectives, both numerical and experimental developments are necessary. With increasing energy prices, the time is right for the multiphase flow community to leverage more than 20 years of research and address challenges facing the fossil fuel energy industries.

In the near term, flow-regime identification, constitutive relations, and simplified models such as 2-D or axisymmetric and statistically steady-state models are the main objectives. Within one flow field, multiple flow regimes exist that exhibit significantly different flow behaviors. A reliable model must provide the ability to analyze such different properties in each region and be able to transition across different regimes. Of course, such results are impossible unless physics-based constitutive relations are available. These relations will have to come from fundamental understanding validated with experimental observations. Hand in hand, numerical models must be used to interpolate and interpret the experimental data, and possibly extend the range of experimental data. Simplified models of real-world problems, e.g. reduced dimensions but nonetheless with fidelity to the salient physical phenomena, can be great examples to garner support from a wide range of communities.

One example of flow regime identification is solid particle size. The solid particles of current interests are those of low Stokes numbers, corresponding to the slurry particles used, for example, in the Fischer-Tropsch synthesis. Larger particles used in ebullated-bed reactors represent a different class of a three-phase system due to Stokes number differences.

Some of the experimental approaches currently available for multiphase flow research include 3-D tomography, MRI, and Gamma-ray particle tracking, as well as extensions of classical fluid dynamical tools such as laser-Doppler and hot-wire anemometry, and particle-image velocimetry. These approaches have been proven to be able to provide a wealth of data for fundamental understanding and numerical model validation, although the difficulty and expense of gaining experimental information deep into an opaque mixture flow remains a severe limitation where much research is needed. To provide confidence in modeling approaches and fully utilize existing experimental understanding, a collaborative effort needs to be in place to define a set of benchmark problems for code validation.

Implicit in the preceding discussion is the close collaboration between experimentalists and CFD software developers. Just as important is close collaboration between academia and industry. Government programs such as the NSF and DOE can be designated to provide the necessary incentives for such collaborations.

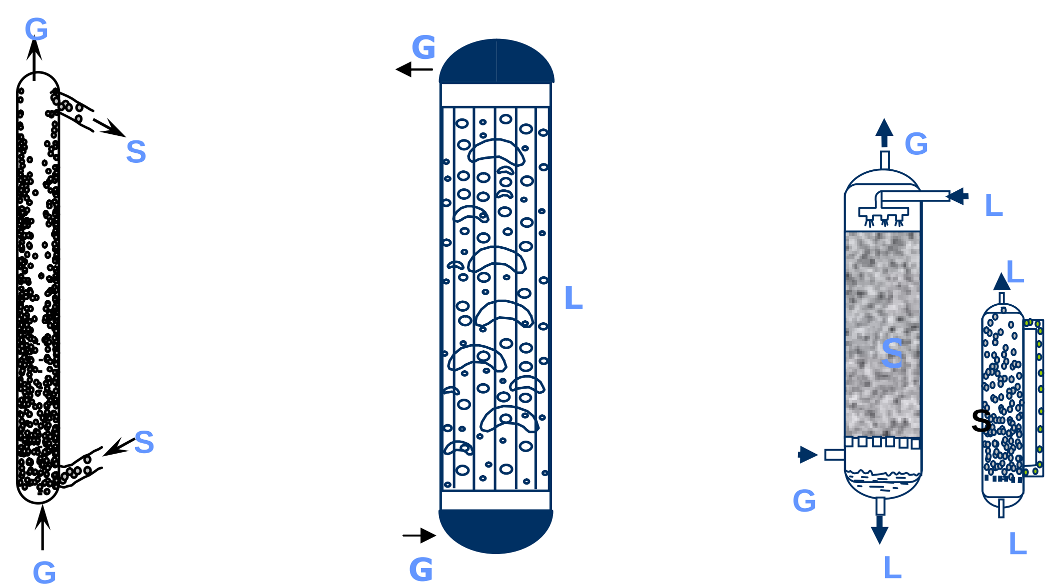
In the mid term, meso-scale models will be a key objective. These multi-scale models are required to accurately describe reacting multiphase flows with heat and mass transfer. A key area of study is to understand multiphase flow behaviors near the wall and at flow inlets and outlets so that accurate boundary conditions can be prescribed. Experimentally, high-pressure and high-temperature conditions must be incorporated in the experimental plan to simulate industrial operations. Enhanced spatial resolution beyond the current 3-mm limit and time resolution will have to be pursued. All requisite data for benchmark problems must be collected and widely shared if meaningful progress is to be made rapidly.

In the long term, the key issue for application is scale-up – from laboratory scale to industrial scale. Numerical codes that embody all available physical understanding must not only capture overall properties such as conversion and process efficiency, but also provide the details to understand the reasons behind the overall observations. Generally, it can be simply stated that by 2015 multiphase flow models should be able to perform at a similar level as single-phase flow models today.

From the fundamental science point of view, it is essential to establish the appropriate structure of mixture flow equations of motion and the constitutive equations for processes which they capture (transport phenomena between the phases, and rate processes such as reaction kinetics). Unlike the equations of single-phase fluid mechanics, these mathematical expressions encompass a vast array of physical situations where there is not a clear separation of scales between the microscale and macroscale physics. As a result, we do not have a guarantee that the **properties** of the material are scale-independent. It is important to establish the limits of approaches which follow from pure fluid mechanics (wherein material properties are incorporated and the equations of motion may then be analyzed on all scales) and thus much prior knowledge may be used, and to probe the physics of systems lying beyond these limits – without this, engineering models will continue to be founded upon uncertain physical foundations and will be trustworthy only within the limited domain for which they were developed.

Action items:

1. Constitute a task force to define benchmark gas-liquid and liquid-solid problems. These problems will guide CFD model development and experimental work.
2. Define two to three research initiatives that address the needs and challenges identified here and solicit funding from appropriate agencies. These programs should be collaborative among different research groups, include both experimental and numerical work, and seek industry participation. The proposed research initiatives should address problems relevant to fuel energy needs.
3. Plan annual/biannual short-duration workshops to disseminate new developments and exchange ideas among the multiphase research community.



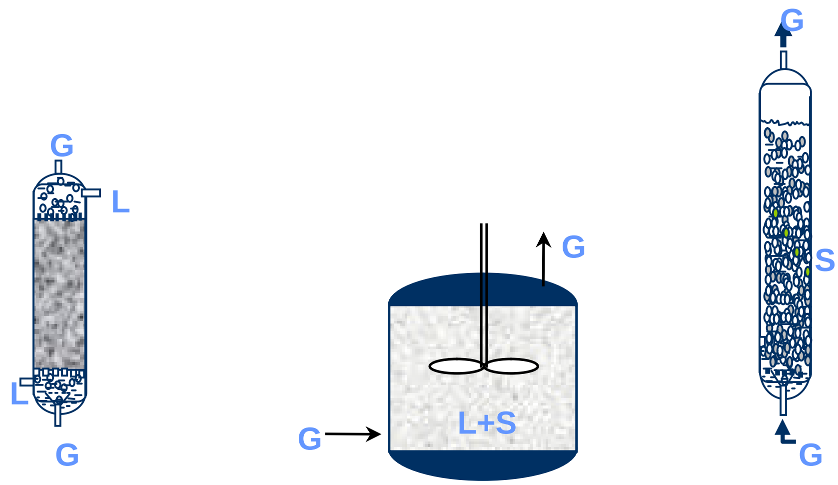
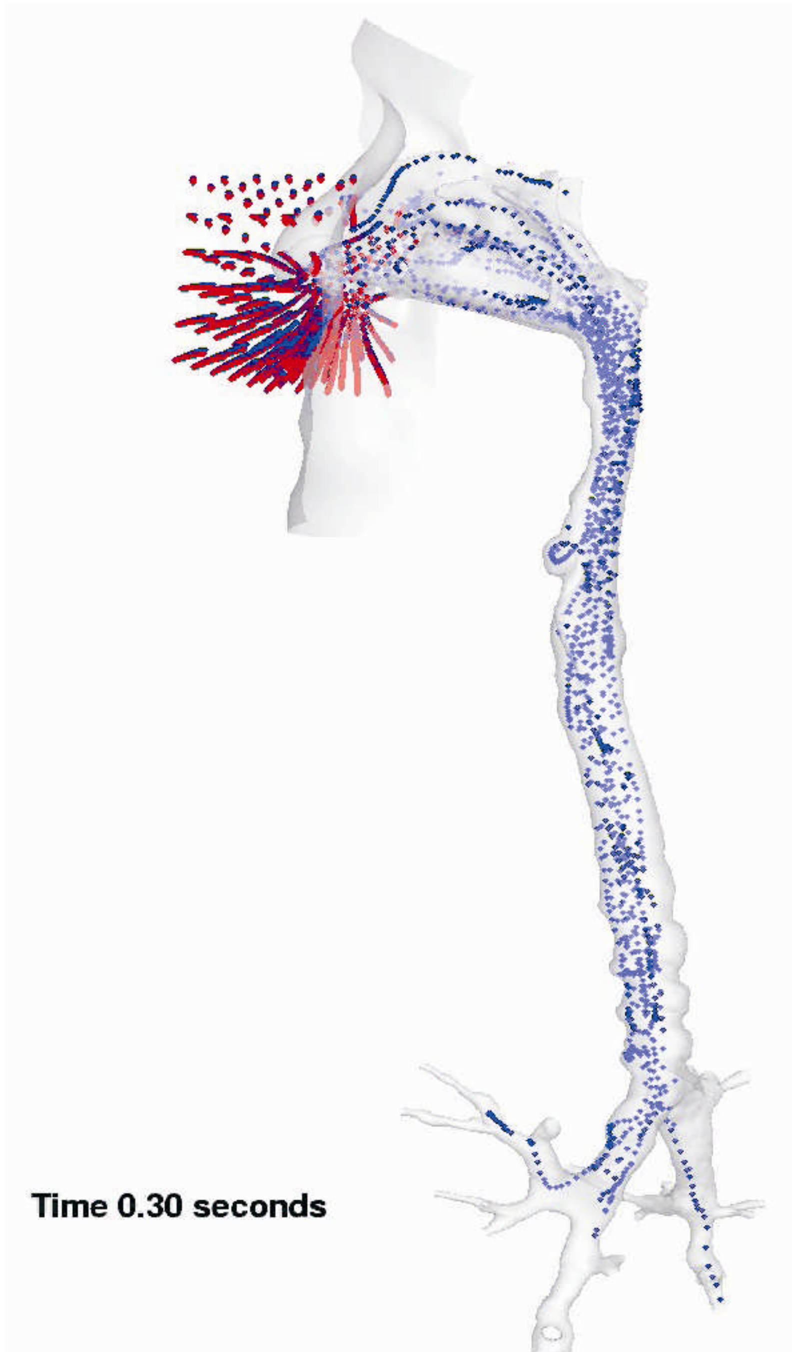


Figure 3.1 Various gas-liquid and gas-liquid-solids systems

♦ *P. Ma, R. Fox, L.S. Fan, J. Morris*



The trajectories of large and small particles being inhaled into the lungs were simulated using the discrete phase model and patient geometry; the project is a first step in the development of a new drug delivery treatment. A. Haidari, Fluent Inc.

4 Computational physics and applications

Findings

The accessibility of ideas and models in multiphase flow is limited by the little amount of data available for model development and validation. A CFD code needs to be developed that allows easy integration of ideas into a platform that supports both Eulerian-Eulerian and Lagrangian-Eulerian frameworks. This code should focus on model development needs such as module integration and user-friendly interfaces. In addition, CFD development in multiphase flow should move beyond the single workstation architecture and embrace a LAN-based computer approach for solving large problems.

Recommendations

Significantly more incentives for fundamental research in the area are needed. Code development needs to be structured to allow easy integration of new ideas into existing commercial codes. Communication efforts from and to all parties need to be enhanced to better implement funding and integration efforts. In short, a formal program needs to be put in place with specific objects in solving industrially relevant multiphase flow problems.

Rationale and Need

Multiphase flow in today's unit operations is not done by choice; it is done by need. The complications often associated with multiphase flows often lead to long start up and operational issues. Merrow [14], of the Rand Corporation, stated that start up of gas-solid unit operations only has a 60% success rate compared to 90% for other unit operations. His findings were based on the survey of 39 U.S. and Canada plants.

This is further complicated by the fact that most multiphase flow unit operations are large and expensive. In addition, multiphase flow often does not scale up in a predictable fashion. Scale-up relationships for many of these units do not exist or can only be used in a limited fashion. Thus, large pilot plants need to be built to provide the scale- up parameters and operational confidences. A large pilot plant, however, results in higher research and development costs and longer implementation times. Many companies are not willing to invest in these costs and times regardless of the economical long-term benefits mostly because the scale-up risk cannot be easily mitigated.

This limited development effort in multiphase flow unit operations has implications that span from energy to environmental issues. A tool that bridges the scale-up gap between concepts and commercial units is needed now more than ever. Many of our fuel, feedstock, and power-producing processes such as Fluidized Catalytic Crackers, fluidized bed combustors, and fluidized bed gasifiers are based on multiphase flow concepts.

Yet, many FCC units have had the same basic design for over 50 years. Breakthrough concepts exist, such as the high-loading FCC process [107] and the Millisecond Fluidized Catalyst Cracker [108], but development efforts are hampered by companies not wanting to take the risk of paying for a novel design. A CFD-based tool that could simulate novel FCC units in a reasonable amount of time could change all that.

Coal fluidized bed combustion is a newer technology that has significantly reduced emissions over existing technology. Yet, even this technology emits more than two times more greenhouse gases[2] than with petroleum and natural gas-based power plants. Additional technologies need to be explored such as hybrid coal combustion and gasification where off-gases are processed as syngas [109]. This hybrid technology adds an additional scale of complexity that may again be a barrier towards commercialization.

Similarly, the chemical industry would also benefit from a scale-up tool for multiphase systems. Such a tool will allow the promotion of advanced reactors and separation systems that use less energy or emit less greenhouse gases. DuPont's maleic anhydride process based on riser technology [110] demonstrates this benefit. Its process reduced carbon dioxide emissions in lieu of making more products. Yet, design issues never observed in the pilot plant led to the demise of this breakthrough technology.

[2] Derived from data of P. Dehmer, Office of Basic Energy Sciences, DOE; In 2002, the U.S. consumed 22.6 Quads of Coal which resulted in 2070 million tons of CO_2 compared to 58.8 Quads of oil and natural gas that emitted 2453 million tons of CO_2.

Even environmental processes would benefit from a fundamentallybased scale-up tool. Three-phase fluidized beds are increasingly being used for aerobic bacterial breakdown of hazardous chemicals. Many large airports are using such a system for bioprocessing their ethylene glycol waste from plane deicing. Yet, the use of these systems for larger waste processing facilities is still limited. The understanding of the scale-up gap from the small airport units to a large-scale bio-treatment facility remains elusive.

These few examples highlight how a fundamentally based scale-up tool, most likely utilizing computational fluid dynamics (CFD), could lead the energy, petroleum, chemical, and environment industries to a resurgence in breakthrough technology in terms of reduced energy consumption, increased energy production, and reduced emissions. Such a tool would bridge the scale-up gap and reduce the development costs that have put the large-scale commercialization of advanced multiphase flow technology on hold for the last 10 years.

Background

There are several commercially available CFD-based codes for modeling multiphase hydrodynamics [111] including FLUENT [112], CFX [113] and Barracuda [114]. CFD codes are also publicly available from U.S. national laboratories including MFIX [115] and CFDLib [116]. Fluent, CFX, MFIX, and CFDLib simulate multiphase flow using Eulerian-Eulerian (two-fluid approach) and Lagrangian-Eulerian (discrete particle treatment, with two-way coupling between the phases; also known as DEM, or discrete element method) frameworks. MFIX is limited to the Eulerian-Eulerian framework but is well-established for fluidized beds and some riser applications. Barracuda uses the Multiphase-Particle in Cell (MP-PIC) method, which is built on a Lagrangian-Eulerian framework, a hybrid between the Eulerian-Eulerian and Eulerian-Lagrangian frameworks. Particles are tracked using the Newtonian physics similar to a Lagrangain framework as is done with discrete-particle methods, except that particle collisions are not resolved individually. Instead, particle stress forces due to collisions are accounted for in the force balance via an Eulerian-type (continuum) constitutive equation for stress. All these codes use Reynolds Average Navier-Stokes (RANS) equations for the Eulerian phases.

These techniques have their strengths and weaknesses. Eulerian-Eulerian codes have the least number of equations (RANS) to integrate, but constitutive equations can be stiff which leads to small time-steps and long CPU times. Furthermore, accurate constitutive relations for non-ideal systems (e.g., polydisperse) are non-trivial to derive at best. With Lagrangain-Eulerian (DEM) and MP-PIC techniques, each particle is tracked individually using a simple force balance based on Newtonian physics. Since each particle trajectory is calculated, particle size distribution can be easily captured but computational requirements are often high. To date, models exceeding one million particles are rare. A commercial FCC riser would require trillions of particles. Thus, DEM codes may be the most rigorousbut are still limited in industrial applications.

The MP-PIC technique is more computationally efficient than DEM since the approximate treatment of collisions precludes the need to detect particles individually, though the accuracy of the predictions are still contingent upon the Eulerian-type stresses employed. For MP-PIC, this CPU requirement is further reduced by treating groups of particles as a parcel or cloud, where the parcel or cloud represents a user-specified number of identical particles with the same velocity. Hence, only a single force balance is required for each parcel as opposed to a single force balance for each particle. For large, three-dimensional problems (where the number of particles is on the order of millions or more), the MP-PIC method tends to be significantly faster than the Lagrangian-Eulerian and Eulerian-Eulerian approaches.

Along similar lines, DEMSolution [117] has developed a DEM code for granular flows (flows in which the role of the interstitial fluid is negligible) called EDEM that can capture some small commercial applications. To model multiphase systems, EDEM can be coupled with FLUENT to provide a gas- or liquid-phase component. EDEM is still limited to less than one million particles owing to its DEM nature.

All of the mathematical frameworks described above (Eulerian-Eulerian, Eulerian-Lagrangian or DEM, and MP-PIC) require a closure model for momentum exchange between the phases, or drag force. Currently, these codes all use some variation of the Ergun or the Wen-Yu equations or the combination of both [118]. Both Ergun [119] and Wen-Yu [120] are based on empirical fits to data from packed beds, settling experiments, or low-velocity fluidized beds. For relatively homogeneous systems, such drag laws may be applicable, but in fluidized beds and risers, particle clustering is commonly observed. The presence of clusters has been detected via the measured slip velocity, where small particles were measured having a higher slip velocity than the predicted terminal velocity [121, p.175]. In other words, the close proximity of small particles (clusters) leads to an increase in apparent “size” of the particle, which is associated with a higher slip velocity between the two phases.

Furthermore, the gas velocity within the cluster is expected to be reduced compared to that flowing around the cluster. Hence, if the existing drag laws (intended for homogeneous suspensions) are applied to a computational fluid grid having both clustered and non-clustered regions (i.e., is characterized by two very different values of solids volume fraction and gas velocity), the resulting drag force will be inaccurate. Such effects have been discussed in detail by Agrawal et al. [53], who suggest a subgrid modeling approach to account for clustering. Alternatively, Yang et al. modified the Ergun and Wen-Yu relationships for particle clustering using an energy minimization multi-scale approach [122], though this approach is semi-empirical in nature.

Another shortcoming associated with the empirical drag laws implemented in existing codes is that they have been targeted at monodisperse, spherical particles. Although ad hoc modifications of these drag laws are used to describe polydispersity, the modifications are oversimplified – e.g., the modifications do not depend on composition of the mixture. Recently, lattice Boltzmann simulations have been used to determine drag force relations specific to polydisperse systems [123]. Lattice Boltzmann simulations involve the solution of the fluid momemtum balance on a grid which is much smaller than the particle size and using a no-slip boundary condition at each particle surface. In this manner, the detailed fluid flow pattern around each particle is known, and thus the drag force can be extracted in a straightforward manner. Hence, the lattice Boltzmann technique involves a greater level of detail than Eulerian-Lagrangian (DEM-based) models, and thus a constitutive relation for drag force is not required, but instead can be extracted directly from the results. Of course, these simulations have even more computational overhead than Eulerian-Lagrangian simulations, and thus cannot be applied directly to systems of practical size.

As alluded above, a tradeoff exists between computational overhead and the required number of constitutive relations needed for closure of the governing equations. Although a drag force is required for each of the methods contained in existing multiphase coding tools, only the Eulerian-Eulerian and MP-PIC method require a closure for solid-phase stresses (which is not the case for Eulerian-Lagrangian/DEM-based methods). In today's CFD packages, particle stresses are modeled using empirical relationships or the kinetic theory [124, 125].

The kinetic theory (based on the kinetic theory of gases) is the most popular approach in which the solids pressure and viscosity is dependent on a granular temperature that represents the kinetic energy associated with random particle motion. On the other hand, Barracuda provides an additional empirical model by Harris and Crighton [126] to describe the stresses required for the MP-PIC method. Both methods have their limitations and require additional development. Namely, the Harris-Crighton expression contains adjustable parameters and is limited to normal components (pressure) of the stress. The kinetic theory is based on first principles and thus does not involve fitting parameters. However, its extension to practical systems (particles with size and/or shape differences) is a non-trivial task.

A final constitutive relationship that merits consideration is gas-phase turbulence. In dense-phase flows, gas-phase stresses (both laminar and turbulent) tend to be significantly smaller than the drag force. Thus, the role of gas-phase turbulence is not expected to be important [59]. However, in dilute flows, the gas-phase stresses may be of similar magnitude as the drag force. Hence, the question to ask is the following: does gas-phase turbulence play a role in the hydrodynamics in systems where both dilute and dense phase flows exists such as the core-annulus profile commonly observed in risers [30] or the freeboard region in fluidized beds?

To summarize, improved modeling of multiphase flow systems such as fluidized beds and risers depends on the development of better drag laws, solid stress models, and possibly gas-phase turbulence models. There are able and available resources to provide the breakthrough needed for commercial application of a multiphase CFD code. Yet, we are hampered by declining funding, legacy computer architectures, and little experimental data for validation. Presented below is a possible roadmap to get multiphase flow research, with an emphais on energy related applications, back on track.

Roadmap Components

On June 6 and 7, team members met to discuss the challenges associated with computational requirements needed to solve an industrially relevant multiphase flow problem. We came up with three metrics over a span of nine years that are needed to meet the "definition of success" for this proposed program. In chronological order, the objectives for each metric were outlined as a scale-up tool capable of modeling:

- A TRDU (transport reactor demonstration unit) -scale gasifier (~200 kg/h coal feed rate) with full 3-D hydrodynamics resolution and particle size distribution by 2009,

- A 12.5 MW transport gasifier (~5,000 kg/h coal feed rate) with full 3-D hydrodynamic resolution, particle size distribution, heat and mass transfer, and phase transformation (liquid atomization) by 2012, and
- A 25 MW transport gasifier (~10,000 kg/h coal feed rate) with full 3-D hydrodynamic resolution, particle size distribution, heat and mass transfer, phase transformation, and heterogeneous reactions by 2015.

All three metrics need to be solved in 24 hours on a single workstation (multiple core and processors allowed) that is standard for its time (2009, 2012, or 2015).

Obviously, these are far-reaching objectives, which can only be achieved with a multi-disciplinary effort that spans academia, industry, and national labs. In order to meet these objectives, seven key areas were highlighted as being critical in achieving the project goal. These areas are funding, education, communications, fundamental physics, numerical methods, code structure, and verification and validation.

Funding

Overall funding for this type of research has decreased in recent years. Consequently, many experts in this field have or are planning to leave the area in search of an area with better funding (such as nanoparticles and biotechnology). Furthermore, the awards often lack enticement for industrial involvement, which often means that the end result is less commercially relevant. Similarly, funding awards are often reduced or delayed, which can reduce the quality and quantity of the resulting research. To achieve the above noted objectives, funding for academic and industrial partners needs to be significantly increased. The best use of funding is expected to be joint university-industrial projects, and should involve experts in the fields that can best contribute to achieving those goals.

Hence, a dedicated project team is needed to insure that funding is available to meet resource requirements. One of the team's objectives would be to frequently communicate with stakeholders on the progress and direction of the program to insure that funding remains available for the duration of the program. The team should consist of notable members from academia, industry, and the national laboratories.

Education

Educational efforts need to span both undergraduate and graduate levels. More emphasis is needed on multiphase flow and numerical methods as part of the mechanical and chemical engineering undergraduate curriculums. On the graduate level, funding needs to include graduate students going to participating companies as interns and individuals from member companies participating in academic research. In addition, support for sabbaticals for both academic and industrial members should be encouraged. This multi-tier approach would generate more interest in the area and promote a better exchange of ideas and concepts.

Communications

Communication between academia, industry, and national laboratories is paramount to the success of the above-noted objectives. To leverage capabilities, collaborate on problems, and coordinate research efforts, a mechanism for communication needs to be developed. Such a communication would suggest "best practices," highlight technology gaps, and disclose code limitations.

One obvious mechanism for this type communication could be done with a dedicated web site (broken down for each track). Such a site can include a "What's New" page, a blog for member-to-team communications, code downloads, code instructions, and documents showing the relational structure of each member with each other (funded partner, collaboration, consultant, etc.). It is important that the web site needs are managed daily to ensure communications with team members and the world is maintained.

A web site could also include documentation and results for various "test cases" to verify and validate modeling efforts. For instance, one test case could be a data set of the pressure drop and bubble size in a fluidized bed containing FCC powder. Other test cases could include axial and radial solids flux data in a riser. Documented residence time distributions (RTD) can also be used as test cases. Details of test cases are presented in the "Verification and Validation" section.

Besides a dedicated web page, a quarterly communication newsletter to all stakeholders should be issued. The newsletter should highlight what has been presented (updated) on the web in a concise fashion. In addition, the newsletter should list recent progress and present a metric on where we are relative to our goals and milestones. Copyright issues need to be addressed such that figures used in the newsletter can also be presented in journals without restrictions.

Finally, it is recommended that annual workshops are implemented such that all team members and potential team members can meet and discuss recent findings, new challenges, and possible gaps. Annual meetings could also provide a venue for readdressing our timeline, goals, and milestones based on recent disclosures. The annual meeting can also be used to approve new data sets as test cases.

Fundamental physics

Although this topic is more relevant to Tracks 1 through 3, there was consensus among Track 4 participants that a fundamental understanding of the physics in multiphase flow, although significantly improved over the last decade, is an area that demands continued attention. The constitutive equations in question include drag and solid stresses (normal and shear). As mentioned above, the drag laws stemming from the work of Wen-Yu [120] and Ergun [119] are based on empirical fits over a wide range of data for relatively homogeneous and monodisperse systems. Using these equations to resolve meso-scale events, such as particle clustering, and/or applying these models in an ad hoc fashion to polydisperse systems, may significantly limit model accuracy. Such an inaccuracy could have a significant impact on resolving gas and solids residence times and reaction rates. Similarly, solid-phase stresses, as derived from the kinetic theory analogy, are typically targeted at uniform, spherical particles. Ad hoc adaptations of these expressions have been applied to more complex systems and incorporated into existing codes, though the inaccuracies associated with such adaptations have not yet been thoroughly analyzed. To overcome the aforementioned obstacles, subgrid models may be obtained via the use of high-resolution simulations. For the case of drag force, lattice Boltzmann simulations, which resolve the detailed flow field around an array of particles, show promise for both monodisperse [127, 128] and polydisperse systems [123]. Similarly, DEM simulations can in principle be used to obtain the continuum quantities required to describe solid-phase stresses for more complex systems [129] (i.e., particles that vary in size, shape and/or density).

Numerical methods

Track 4 did not discuss specific numerical methods involving the spatial and temporal integration of Lagrangian-Eulerian or Eulerian-Eulerian equations. Instead, the focus was directed more at the development and incorporation of subgrid models. Most of today’s codes are based on governing equations using predefined, and often empirical, constitutive equations for closure of the drag coefficient, solids pressure, solids viscosity, and Reynolds stresses. However, the empirical nature of these constitutive equations may be limiting modeling accuracy.

One way to limit these inaccuracies is to calculate the closure terms from higher-resolution simulations as described above for drag (via lattice Boltzmann simulations) and solid-phase stresses (via DEM simulations). Thus, various closure properties could be based on a subgrid scale first before the calculations of the larger domain are started. Such a method was developed for reaction schemes in turbulent flows by Steve Pope of Cornell University [72].

Thus, if we go back to the drag force example in the previous section, the drag can be calculated for a particle with respect to its nearest neighbors (and their densities, sizes, and shapes) over a range of gas and particle velocities in a small, well-defined domain. These values then can be stored in a manifold such that they can be recalled, as needed, during the computation of the larger domain.

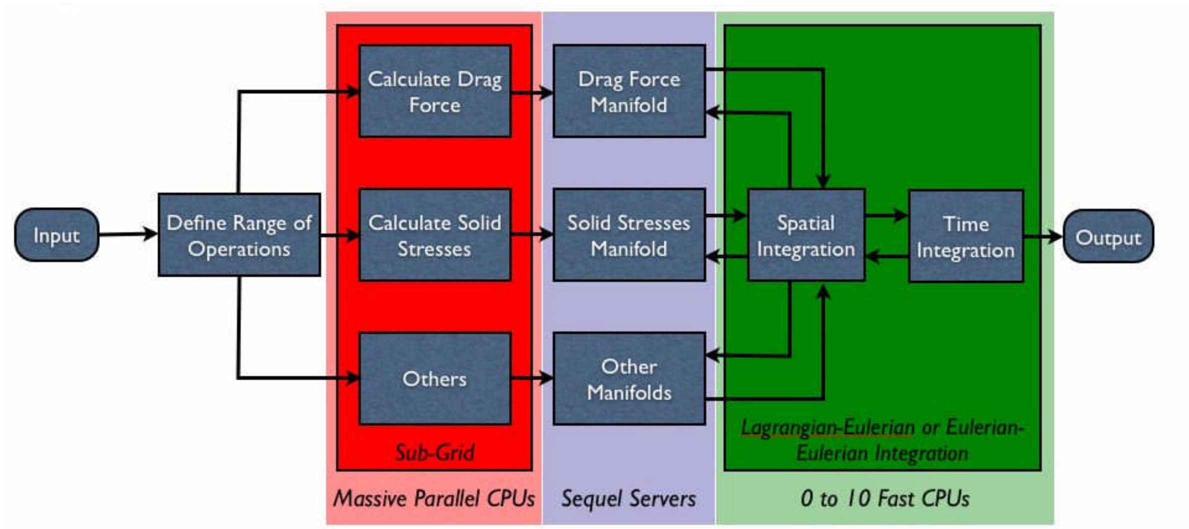


Figure 4.1: Proposed flow diagram for integration of sub-grid models.

Figure 4.1 provides an example of this method. The drag forces and solids stresses are calculated over the entire range of expected factors and responses. For drag, the response would be dependent on the range of gas and particle relative velocities, particle loading, density, size, and shape. Similarly, the solid stresses responses (solids pressure and viscosity) would be dependent on the ranges of velocity, solids loading, particle properties, and predicted shear rates and or granular temperature. Other properties can be calculated and stored in a manifold as well such as reaction rates, gas turbulent properties, and Coulombic forces (as an example).

Each saved response of the sub-grid model is stored relative to all factors. The spatial integrator can summon these values for the factors defined by the integrator. A sequel server (SQL) may be a suitable means of storing manifolds.

Pre-calculating the responses of the sub-grid models offers the advantage that each sub-grid model can be calculated on massively parallel clusters.

Since sub-grid models used a small, predefined grid over a predefined range of factors, the computation is explicit and independent of time-dependent responses.

Once the manifolds are calculated, the spatial and temporal integration, where responses are implicit, can be calculated on a typically clustered machine (~10 CPUs). Having more CPUs may not be advantageous, as most codes today do not see a significant increase in solution speed with more than ten processors (limited parallelization capabilities). However, since the stiffness of the governing equations has been mitigated to the manifolds calculations, the integration of the RANS equations would be less of on issue here and simulation times would be reduced.

Code structure

In order to promote the rapid development of fundamental codes, a CFD engine needs to be freely available. Such an engine would contain a variety of spatial and temporal integrators with the ability to link in various constitutive equations. This engine should be capable of Lagrangian-Eulerian and Eulerian-Eulerian calculations, as well as relevant hybrids. Figure 4.2 gives a depiction of this type of CFD framework.

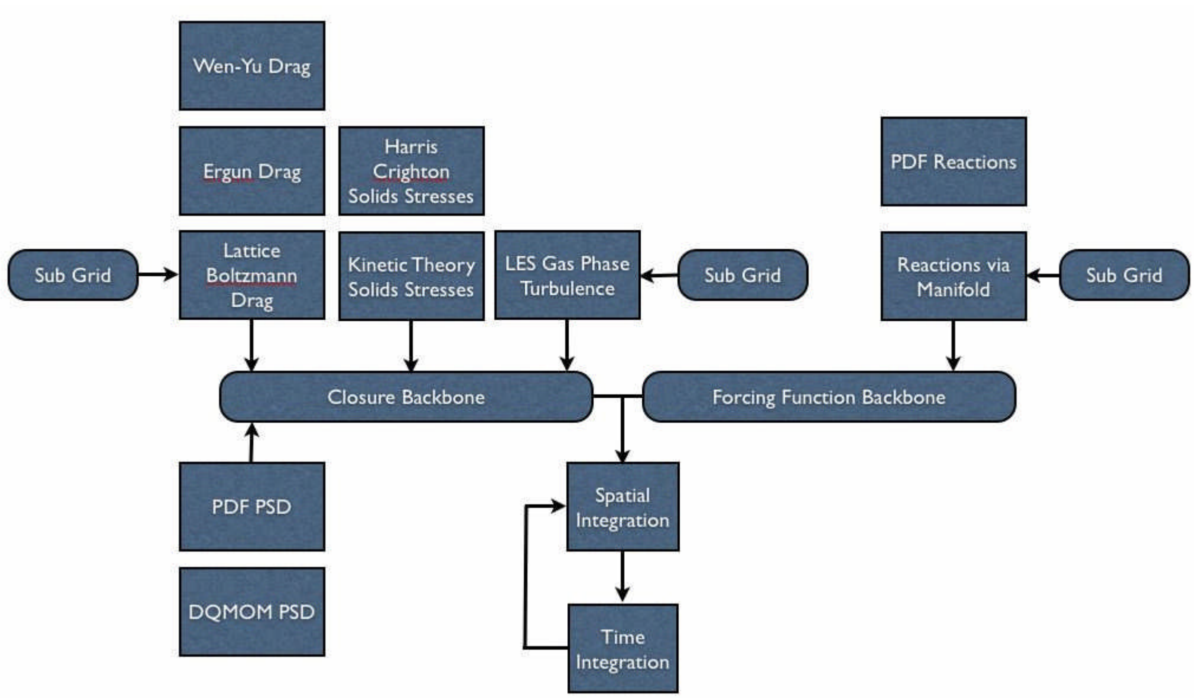


Figure 4.2: Possible modular framework for a developer-based CFD engine.

The developer-based CFD code, DBCFD, would provide the spatial and temporal integrators with hooks for adding closure models and forcing functions (RHS). These hooks need to be defined and standardized such that adding a closure model would be as simple as adding/linking a module. A similar approach can be taken for the spatial and time integrators. Factors and responses from each computational cell should be done in a single defined matrix. Although the matrix would be large, it would be less confusing and standardized across all types of modules. A similar method is used for modular development with ASPEN Plus using CAPE-OPEN.

The DBCFD should be open-sourced so developers have full access to the CFD engine. Open-sourced software has the advantage of continuous improvement which needs to be inherent to this research program. However, an oversight process needs to be in place to insure improvements are value added and verified. Both CFDLib and MFIX are open-sourced and have done a good job evaluating and improving their codes.

Ease of use is one factor that needs attention with the proposed DBCFD engine. The engine needs to run on all platforms and be as user friendly as possible. It is recommended that the DBCFD engine (and GUI) is written in JAVA to easily support multi-platform capabilities. CFDLib has already been ported as a JAVA code with success [130]. The JAVA-based CFDLib was reported at running at only half of the speed as the Fortran-based CFDLib code. With additional code developments and advances with JAVA, we expect that a JAVA-based code will be comparable in speed to the standard CFDLib code written in Fortran.

Figure 4.3: FoamX Case Manager

If possible, the DBCFD engine should be GUI-based to manage modules, inputs, and outputs. OpenFOAM uses a GUI-based CFD system that is a good example of this called the "FoamX Case Manager," as shown in Figure 4.3. The DBCFD code would have a module manager that would allow the incorporation of various constitutive equations as well as various integrators (SuperBee, compressibility, etc).

The DBCFD GUI should also handle grid import, data export, and basic post processing. Sophisticated gridding such as hexmeshing and automeshing should be handled from third-party software vendors. Similarly, sophisticatd post-processing can also be handled with third-party applications. In addition, we should leverage the gridding importing algorithms from CFDLib and the post-processing capabilities of MFIX. In addition, DBCFD should handle advanced gridding from file imports of STL and IGES formats and provide output files compatible with visualization software Ensight and Gmv.

Verification and validation

The DBCFD code should be treated like the development of a commercial code. All changes and improvements need to go through a verification process. Thus, an oversight committee will be needed for the management of the DBCFD code. This committee will be responsible for insuring that any formal improvement to the DBCFD engine will involve a formal verification process.

Similarly, validation needs to have a formal process managed by an oversight committee. Unfortunately, there are only a few data sets available for model validation, as noted above. In order to standardize the validation process, data sets from riser, fluidized bed, dense-phase conveying, and hopper flow problems need to be available to all developers. DEM-based simulations of relatively small systems can also be used for validation of Eulerian-Eulerian models. The oversight committee should determine those datasets, which are the best tests for each of the constitutive models described above (drag, solid-phase stress, gas-phase turbulence, etc.)

This oversight committee should identify at least three validation data sets from each fluidization regime (bubbling bed, turbulent bed, riser). Riser data should consist of high and low solids fluxes with high and low gas velocities such that at least one case has upflow at the walls while the remaining data sets have downflow at the walls (or vice versa). Fluidized bed data should range from bubbling fluidized beds to turbulent fluidized bed with particle size distributions ranging from Geldart Groups A and B. Dense-phase conveying data should include dune and slug flow regimes. Hopper data should include both mass and funnel flow regimes with dilation.

Data sets need to be complete and include factors (inputs) concerning particle size distribution, particle density, particle shape, gas density, gas viscosity, temperature, pressure, moisture content, electrostatics, specific equipment configuration, superficial gas velocity, purge gases, and solids feed rate. Responses need to be equally precise and detailed (local measurements as opposed to bulk) and include all components of gas velocity and solids fluxes, axial pressure drop (with a representative sampling), particle size distribution profiles (axial and radial), attrition profiles, gas residence time distributions, bubble sizes and rise velocities, transient pressure responses via power spectra, and if possible solids residence time distributions. In addition, the accuracy and reproducibility of each measuring technique need to be documented (including particle size sampling and analysis). Similarly, data acquisition information such as sampling rates, sampling times (i.e., buffer), and subsequent calculations need to be clearly disclosed. In short, it is imperative that experimental data sets are characterized as completely as possible – all physical parameters needed for model input should be measured directly, and the flow field variables to which model predictions will be compared should be measured locally (to obtain radial, axial, etc. profiles).

Having a complete set of data to be used specifically for validation will streamline development efforts and promote more rapid model development. With everyone working with the same data sets (but not limited to), the exchange of ideas and critique of model development will be better facilitated.

Leveraging and Sustainability

A project with such far-reaching goals needs to have a substantial leveraging and sustainability plan. For model and code development, this process is mostly dependent on communications. A formal process needs to be in place for both resource and technical management involving all team members. A clear description of realistic deliverables needs to be formally written yet this document needs to be flexible enough to allow additions, modifications, or deletions of deliverables. Similarly, a path forward needs to be documented that highlights not only the next quarters,but also the next year and five-year period (this document should also be one of the deliverables).

Finally, the funding structure and requirements need to be clearly disclosed. A cut in promised funding on any project for reasons other than performance has a disastrous negative effect on even a reduced set of deliverables (as the effort put toward a large-scale research effort may not be applicable to a smaller-scale effort).

Similarly, technical exchanges need to be clear and open. A format needs to be in place that promotes the frequent exchange of ideas and open discussion of hypothesis and theories. This format needs to consist of several communications methods including frequent (biannual, annual) meetings, web pages, blogs, newsletters, and refereed publications. NETL's MFIX website is a good example of how some of these attributes can promote technical advances in code development.

Education needs to be a top priority for such a long-term project timeline. Success is dependent on leveraging and sustaining the best and brightest on the team. A good educational program will insure the best and brightest are interested in this research area.

Proposal funding should be based on the approval of a technical committee consisting of notable members from industry, national laboratories, and academia in the field. Funding should be based on merit in relevant expertise and past performance with deliverables. Awards should be publicized along with a disclosure of the objectives, deliverables, and milestones. Fair distribution of funding based on merit is critical in sustainability as it will keep the best and brightest involved in this program.

If a project is managed to promote open communications of resources and technology, leveraging and sustainability can be self-propagating. Projects often fail because of poor management and not because of technical obstacles. Having the right project management team and technical committee that promote the use of effective communications tools can be the difference between success and failure.

Summary and Principal Recommendations

The team agreed that model and code developments are limited by the availability of data that focuses on the fundamentals of drag forces and solid stresses (pressure and friction). Recently, available and targeted funding in this area has been decreasing, and we do not expect the project goals to be fulfilled without a change in the funding situation.

The team outlined three metrics (proposed) against which the project can be assessed. These metrics are as follows:

- A TRDU-scale gasifier (~200 kg/h coal feed rate) with full 3-D hydrodynamics resolution and particle size distribution by 2009.

- A 12.5 MW transport gasifier (~ 5,000 kg/h coal feed rate) with full 3-D hydrodynamic resolution, particle size distribution, heat and mass transfer, and phase transformation (liquid atomization) by 2012.

- A 25 MW transport gasifier (~10,000 kg/h coal feed rate) with full 3-D hydrodynamic resolution, particle size distribution, heat and mass transfer, phase transformation- and heterogeneous reactions by 2015.

All three cases need to be solved in 24 hours on a single workstation (multiple core and processors allowed) that is standard for its time (2009, 2012, or 2015). These are significant objectives and can only be achieved with a multi-disciplinary effort that spans academia, industry, and national labs.

Seven key areas were highlighted as being critical to achieve the above noted objectives. These areas are the following:

- Funding: Additional and targeted funding is needed to reinvigorate this area of research that has suffered from recent decreases in available funding.

- Education: A project with such goals and duration needs to have an educational program in place such that good ideas and people resources are never in short supply.

- Communications: Team dynamics is dependent on communications. For projects involving diverse geography, communications needs to span several medias including web pages, newsletters, updates, and on-site meetings.

- Fundamental physics: The CPU engine needs to be designed such that new constitutive equations (or forcing functions) can be easily tested.

- Numerical methods: In order to do calculations overnight, sub-grid models may have to be computed before the RANS integration. Constitutive sub-grid models can be calculated on a massively parallel cluster with values stored in a sequel server and RANS (or DEM) integration on a multi-core workstation.

- Code structure: The code needs to be written in a language that is platform-independent, such as JAVA. Code structure needs to be designed such that various components (constitutive, forcing functions, and integrators) can be easily added to the CFD engine

- Verification and validation: Both are important and should be one of the most important metrics with this program.

It is critical that the project management team focus on all these efforts with assigned responsibilities and accountabilities, while strongly emphasizing communications and education. We feel that the 2015 target is achievable, but only with a strong and diverse management team that knows how to stimulate ideas, promote leveraging, manage funding needs, develop sustainability, and foster motivation. To quote Lee Iacocca, *"Motivation is everything. You can do the work of two people, but you can't be two people. Instead, you have to inspire the next guy down the line and get him to inspire his people."*

♦ *R. Cocco, C. Hrenya*

5 Technology Roadmap

Workshop discussions in each of the four tracks produced a set of near-term, mid-term and long-term research needs to achieve the goal *that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants.* These needs include further developments in theory, experiments, computational algorithm and code development and validation. The research needs in the four tracks were then put together in an effort to identify themes that cut across the various tracks. An initial presentation on such integration was prepared by Professors Dimitri Gidaspow and Sankaran Sundaresan. They observed that the workshop identified several issues that cut across the four tracks, which can be grouped into four categories:

- Numerical algorithm and software development
- Theory and model development
- Physical and computational experiments
- Communication, collaboration and education

The information from the four track reports is summarized below grouped into the above four categories and the category of benchmark cases identified during the work shop.

	Near-Term (by 2009)	**Mid-Term (by 2012)**	**Long-Term (by 2015)**
A. Benchmark Cases	1. High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics-only simulation of transport reactor at TRDU-scale (200 kg/h coal feed rate) to run on 2009 computer cluster overnight. 2. Develop reduced-order, approximately real-time model of the above case that can be linked to process simulators.	1. High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics with heat and mass transfer simulation of transport reactor at a scale of at least 12.5 MW (or 5,000 kg/h coal feed rate) to run on 2012 computer cluster overnight. 2. Repeat Near-Term Case 1 with addition of considering density variations (multiple solids species) 3. Develop reduced-order, approximately real-time models of Mid-Term Case 1 that can be linked to process simulators	1. High-fidelity, transient, 3-D, two-phase with particle size and density variations, hydrodynamics with chemical reactions simulation of transport reactor at a scale of at least 25 MW (or 10,000 kg/h coal feed rate) to run on 2015 computer cluster overnight. 2. Develop reduced-order, approximately real-time models of Long-Term Case 1 that can be linked to process simulators
B. Numerical Algorithm and Software Development	1. Improve numerical stability and efficiency of parallel computations. 2. Develop detailed protocol for the integration of various codes; e.g., Common component architecture for linking software components. 3. Develop coarse-grained (filtered) two-fluid models. 4. Develop reduced order models from accurate computational results for use by design engineers. 5. Demonstrate that the models correctly capture the effect of temperature and pressure.	1. Demonstrate that the models are able to predict the transition in the fluidization behavior when the particle properties change from Geldart group B to group A. 2. Develop initial fully coupled reactive multiphase flow model. 3. Develop automated procedure to coarsen hydrodynamic (non-reactive or with simple reactions) results from CFD for use with more complex reaction networks. 4. Develop in-situ adaptive tabulation of chemical reaction rates for heterogeneous reactions and couple with full CFD simulation for reactive	1. Integrate developments to complete fully coupled reactive flow model for industrial-scale reactors capable of handling a range of mesh sizes with reasonable run times. 2. Solve numerical stiffness problems in multi-physics simulations (reaction, radiation, density jumps, etc) 3. Demonstrate that models that can correctly model the effect of internals such as heat transfer tubes. 4. Investigate the use of the detailed models for scale up and process control (See Table 1.4).

	Near-Term (by 2009)	Mid-Term (by 2012)	Long-Term (by 2015)
	6. Identify the deficiencies of the current models, assess the state-of-the-art, and document the "current best approach". 7. Identify a standard approach for multiphase flow code verification. 8. Develop a plan for generating validation test cases, identify fundamental experiments, and identify computational challenge problems.	flows. 5. Develop models and codes that explicitly recognize and account for the micro/meso/macroscale picture that is emerging from studies at these different scales. 6. Develop software framework that allows multiple codes (open-source and commercial) to work together. 7. Solve numerical issues with the treatment of PSD (e.g., DQMOM).	
C. Theory and Model Development	1. Develop fundamental aspects of stress and flow fields in dense particulate systems (See Table 1.1). 2. Develop drag relations that can handle particle size and density distributions and are applicable over the entire range of solids volume fraction. 3. Develop stress relations for dilute poly-disperse systems. 4. Formulate proper boundary conditions for multiphase flow systems. The wall boundary condition must capture key effects such as the solids flux distribution near a wall. Exits – how to handle solids versus	1. Develop continuum descriptions of dense particulate systems (See Table 1.3). 2. Handle the transition from regimes in which the particles are in enduring contact to regimes in which the particles are in collisional contact. 3. Develop methods to model adsorption/desorption and heterogeneous chemical reactions. 4. Determine the significance of electrostatic forces and van der Waals (cohesive) forces on hydrodynamics and develop appropriate models. 5. Develop the theory to model liquid feed injection and	1. Model particle deposition and re-suspension, which includes the effect of particle size distribution. 2. Model particle attrition and agglomeration, and fragmentation of coal. 3. Account for particle dispersion in solid-fuel injectors and gasifiers. We need to simultaneously account for particle dispersion as well as fluctuating kinetic energy. 4. Determine the significance of gas emanation from particles (via chemical reactions) on overall hydrodynamics and develop appropriate models. 5. Develop model for erosion of

	Near-Term (by 2009)	Mid-Term (by 2012)	Long-Term (by 2015)
	gas boundary conditions. Use DEM or other techniques to resolve issues. 5. Understand the cause and effects of particle clustering. The effect of particle clustering on drag, collisions, and gas-phase turbulence modulation are needed. 6. Development of constitutive relations for continuum models from discrete models such as DEM or LBM, which are based on fewer assumptions than the continuum approach. 7. Identify flow-regimes in gas-liquid and gas-liquid-solids flows and develop appropriate constitutive relations and simplified models.	subsequent evaporation of liquids. 6. Model flow regime transitions in gas-liquid flows; e.g., the transition in a bubble column from “bubbly” to “churn turbulent” regime. 7. Develop radiation model for particle-particle and particle-wall heat transfer. 8. Develop constitutive models for non-spherical particles. 9. Develop multiphase turbulence models that incorporate fluctuations in the volume fraction. 10. Consider the effect of lubrication forces in particle-particle interactions.	walls or internals by particle impact. 6. Solve several fundamental theoretical challenges in mathematical formulations of multiphase flow: resolution of ill-posedness of continuum multiphase flow equations, eliminating the need to time-average the solution of continuum models for statistically steady problems.
D. Physical and Computational Experiments	1. Provide detailed circulating fluidized bed data on at least two scales (~0.15 m and ~0.6 m diameter vessels). The experiments must have well-defined entrance, exit, and boundary conditions and should report detailed data for local pressure, velocity of solids and gas, solids fraction, fluctuations, cluster sizes, and	1. Define material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements (See Table 1.2). 2. Use large flow facility to elucidate the effect of particle size distribution on flow. Determine lateral distribution of	1. Full-field visualizations of rotational motions of spherical and non-spherical particles in quasi-2-dimensional situations and 3-d tracking of particles in semi-dilute situations (volume fractions of up to 10 or 15%) that takes into account: frictional interactions, bidisperse or polydisperse grains, and non-

	Near-Term (by 2009)	Mid-Term (by 2012)	Long-Term (by 2015)
	solids flux. 2. Develop well-calibrated, non-intrusive probes to simultaneously measure the velocity and volume fraction of different phases. Planar flow field, rather than point-to-point traverses, is required (e.g., measure radial solids concentration in riser using MRI). 3. Develop experimental techniques for gaining information from deep into opaque multiphase mixtures. 4. Measurements of near wall phenomena to establish wall boundary conditions. 5. Small-scale experiments to provide data to improve and check sub-models; e.g., simultaneously measure drag in gas-solids flows as well as gas and solid velocities (slip). 6. Develop standardized experiments or detailed simulations (discrete element or lattice Boltzmann) or a combination of both to derive a custom drag formula for a given powder.	particle sizes and segregation. 3. Measure spatial variation of PSD. 4. Conduct multiphase chemical reactor experiments with detailed measurements (e.g., ozone decomposition in fluidized beds). 5. Determine the importance of flow- generated electrostatic forces on dilute gas-solids flows for both cold and hot (process) conditions. 6. Measure flow fields in the presence of obstacles, such as heat transfer tubes, baffles, etc. 7. Develop measurement techniques for high pressure and temperature bubble columns. 8. Collect detailed data from 3-D tomography (MRI, X-ray, capacitance imaging etc.)	spherical grains.

	Near-Term (by 2009)	Mid-Term (by 2012)	Long-Term (by 2015)
E. Communication, Collaboration, and Education	1. Constitute a task force to define benchmark gas-liquid and liquid-solids problems, which will guide CFD model development and experimental work. 2. Establish a communications network for the multiphase research community, which may include newsletter, web page, and regularly scheduled seminars and workshops. 3. Education: Develop curriculum for modular university courses; train adequate number of graduate students in this area; develop on-line instructional modules.	1. Establish communication between different entities working on open source multiphase flow codes. 2. Develop challenge problems for multiphase flow with heat & mass transfer and chemical reactions.	

Glossary

AspenPlus	Commercial steady-state process simulation software (http://www.aspentech.com/brochures/aspenplus.pdf).
ASCI	Advanced Simulation and Computing Initiative [20].
ASTM	American Society for Testing Materials.
BARRACUDA	Commercial CFD software (www.barracuda-cpfd.com/welcome.html).
CAPE-OPEN	Computer Aided Process Engineering – Open Simulation Environment Interface definitions for exchanging information with process simulation software (www.colan.org).
CCPI	Clean Coal Power Initiative.
CFB	Circulating Fluidized Bed.
CFD	Computational Fluid Dynamics.
CFDLib	CFDLIB is the Los Alamos Library of computer codes capable of solving a wide range of CFD problems (www.lanl.gov/orgs/t/t3/codes/cfdlib.shtml).
CFX	Commercial CFD software (www.ansys.com/products/cfx.asp).
CMFR	Collaboratory for Multiphase Flow Research. A planned organization consisting of NETL, Carnegie Mellon University, University of Pittsburgh, and West Virginia University for conducting collaborative research in multiphase flow.
COE	Cost of electricity.
Collaboratory	A term perhaps coined by Professor William Wulf (University of Virginia) by blending *collaboration* and *laboratory* to describe the method that may enable researchers, thousands of miles apart, from different organization to work together in a “laboratory without walls” by using information technology.

	http://www.worldwidewords.org/turnsofphrase/tp-col1.htm
CPU	Central processing unit of a computer.
CSP	Computer Singular Perturbation.
CSTR	Continuous Stirred Tank Reactor.
DBCFD	Developer-Based CFD engine. (see Figure 4.2).
DEM	Discrete Element Model.
DNS	Direct Numerical Simulation.
DPM	Discrete phase model. A method in which the motion of individual (or group of) particles is tracked without considering particle collisions.
DQMOM	Direct quadrature method of moments.
DTI	Department of trade and industry (U.K.).
EDEM	Commercial DEM software from DEMSolution [117].
E-E Model	Eulerian-Eulerian model. A model in which the gas and granular material are treated as interpenetrating phases.
ESP	Electrostatic precipitator. Used for removing particulate material from flue gas.
FCC	Fluid Catalytic Cracking reactor.
FLUENT	Commercial CFD software (www.fluent.com).
Geldart Group	Classifies powders into groups A, B, C, and D based on particle diameter and density. See diagram on page 22 [121 pp. 33-51.]
Gmv	Grid Mesh Viewer. http://www-xdiv.lanl.gov/XCM/gmv/GMVHome.html
GUI	Graphical User Interface.
HHV	Higher heating value.

IFPRI	International Fine Particle Research Institute.
IGES	Initial Graphics Exchange Specification is neutral exchange format for 2-D or 3-D CAD product models, drawings, or graphics.
ILDM	Intrinsic Low-Dimensional Manifolds, a method for reducing the system of chemical kinetics.
ISAT	Insitu Adaptive Tabulation.
ISO	International Standards Organization.
LAN	Local Area Network.
LBM	Lattice Boltzmann Method.
LES	Large Eddy Simulation.
MFIX	Open source gas-solids multiphase CFD software developed at NETL (www.mfix.org).
MP-PIC	Multiphase-Particle in Cell method.
MRI	Magnetic Resonance Imaging.
NASA	National Aeronautics and Space Agency.
NIST	National Institute of Standards and Technology.
NETL	National Energy Technology Laboratory.
NSF	National Science Foundation.
OpenFOAM	Open source CFD software. (http://www.opencfd.co.uk/openfoam/).
PBM	Population Balance Model.
PIV	Particle-Image Velocimetry.
PSD	Particle Size Distribution.
PSDF	Power Systems Development facility at Wilsonville, Alabama.
RANS	Reynolds-Averaged Navier Stokes equations.

Regolith	The layer of loose, heterogeneous material covering solid rock. Regolith is present on Earth, the Moon, some asteroids, and other planets.
RTD	Residence Time Distribution.
SciDAC	Scientific Discovery through Advanced Computing [21].
SCR	Selective Catalytic Reduction. A method for reducing NOx in flue gas.
STL	Stereolithography format for graphics.
SQL	Structured Querry Language: language for updating a relational database, or retrieving data from it.
TRDU	Transport Reactor Development Unit at University of North Dakota (http://www.undeerc.org/rnd/equipment/trdu/default.asp).
Validation	The process of confirming that the equations are (physically) accurate [24].
Verification	The process of confirming that the equations are numerically solved accurately [24].

Appendices

A. Workshop Agenda

June 6, 2006

Time	Title	Speaker/Leader
7:30-8:15	Breakfast/Registration	
8:15-9:00	Welcome and NETL overview	A. Cugini (Acting Director, ORD-NETL)
9:00-9:15	Workshop objectives and agenda	M. Syamlal (ORD-NETL)
9:15-9:45	Dense gas-solids flows and Granular flows	P. Mort (P&G) J. McCarthy (U. Pittsburgh)
9:45-10:15	Dilute Gas-Solids Flows	R. Patel (Exxon-Mobil), S. Subramaniam (Iowa State U.)
10:15-10:45	Break	
10:45-11:15	Liquid-solids/Gas-liquid flows	P. Ma (Air Products) R. Fox (Iowa State U.)
11:15-11:45	Computational Physics and Applications	R. Cocco (PSRI) C. Hrenya (U. Colorado)
11:45-12:00	Organization of tracks	Track chairs
12:00-1:00	Lunch	
1:00-3:00	Parallel technical track breakout sessions	Track chairs
3:00-3:30	Break	
3:30-4:30	Parallel technical track breakout sessions	Track chairs
4:30-5:00	Day's wrap up, information for next day	

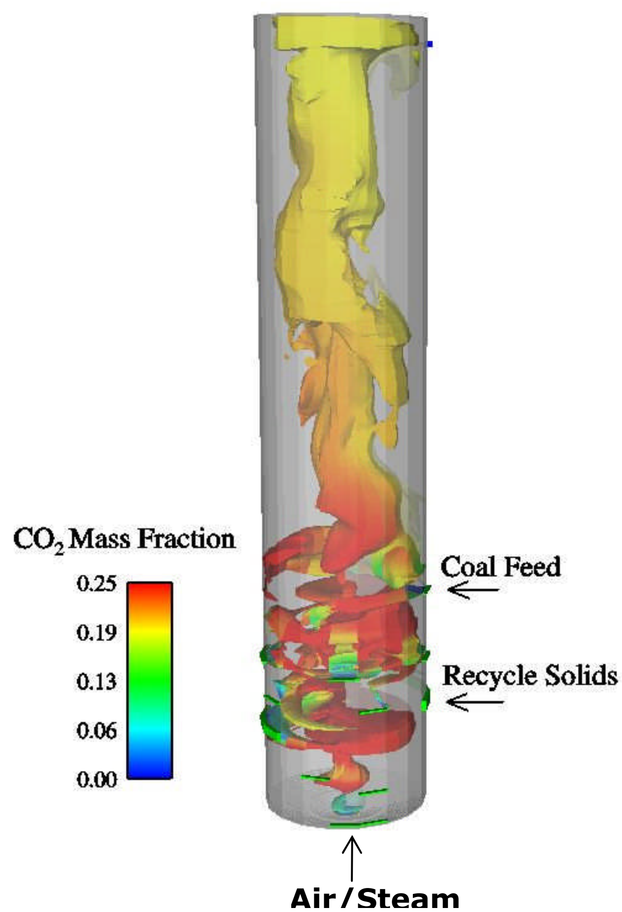
June 7, 2006

Time	Title	Speaker/Leader
7:30-8:00	Breakfast	
8-8:15	Recap workshop objectives and day's agenda	
8:15-9:45	Presentations on the results of 4 breakout sessions by track chairs and moderated general discussion	T. O'Brien (NETL)
9:45-10:15	Break	
10:15-11:15	Integration of technical track presentations	D. Gidaspow (IIT) S. Sundaresan (Princeton)
11:15-11:45	Vision for a Collaboratory on Multiphase Flow Research: presentation and discussion	W. Rogers (NETL)
11:45-12:00	Conference wrap up	
12:00-1:00	Lunch (on your own)	
1:00-2:30	Discuss follow up action items; Attended only by the organizing committee.	Track chairs and discussion leaders
1:00-2:30	Optional NETL lab tour	

B. NETL Uses Multiphase Model for Coal Gasifier Design

Coal gasification is an efficient and environmentally acceptable technology that can utilize the vast coal reserves in the United States to produce clean affordable power and reduce dependence on foreign oil. Coal and other carbon-containing materials can be gasified to produce a synthesis gas. This syngas can be fed to a turbine to produce electricity or used in a number of petrochemical applications to produce fuels, chemicals, fertilizers, or other industrial gases. Given the tremendous potential of coal gasification, understanding the process is a critical need and is being addressed by the Power Systems Development Facility (PSDF) in Wilsonville, Alabama. The PSDF is a joint project between the U.S. Department of Energy, Southern Company, and Kellogg Brown & Root (KBR) to carry out research and development on advanced power systems and components. The centerpiece of this project is the development of the transport gasifier. The transport gasifier has higher throughput, better mixing, and increased heat and mass transfer rates compared to other conventional technologies.

To better understand the complex interactions between the gas and solids inside the transport gasifier and to optimize the process and design, the U.S. Department of Energy's National Energy Technology Laboratory (NETL) has been actively involved in developing and applying computer simulations of the gasifier. For over 20 years, NETL has been committed to the use of physics-based computer simulations to understand multiphase flow problems. This commitment has resulted in the development of the MFIX (Multiphase Flow with Interphase eXchanges, www.mfix.org) code, which is



Solids volume fraction isosurfaces colored by CO_2 mass fraction. Simulated using MFIX by C. Guenther, NETL.

internationally recognized as one of the premier multiphase codes available to researchers. NETL has also been developing a detailed chemistry module for the coal gasification process. For the last three years, researchers at NETL have been using MFIX with the coal gasification chemistry module to simulate the transport gasifier at the PSDF. This model is a transient three-dimensional model capable of providing velocity, temperature, pressure, and gas/solids species composition anywhere inside the reactor. To validate the gasifier model, NETL researchers have been using available experimental data at the PSDF. Axial temperature profiles, incremental pressure differences, exit syngas composition, and axial gas samples have all been used to validate the MFIX model. The model has been validated for both bituminous and sub-bituminous coals under air and oxygen-blown conditions.

An important factor that led to the success of this effort was the continual communication of the simulation results with the gasifier developers. Regular review meetings at PSDF have been conducted and modeling results have been presented at each of these meetings. Acceptance of the modeling results at PSDF was initially difficult. However, the acceptance dramatically improved when in two instances simulation results showed unexpected phenomena that were subsequently verified. One, the simulations showed that oxygen reached the upper region of the mixing section. The gasifier developers had expected that all the oxygen would be consumed by the recycled char in the lower region of the mixing section. This prediction was later verified with experimental measurements. Two, the calculations showed high concentration of CO and solids in the upper part of the riser, above the exit. This prediction was also later confirmed with experimental measurements. These convincingly showed the gasifier developers that the model does not merely reproduce what is already known, but provides information on unobserved phenomena.

Another difficulty that the design engineers often have is with the large computational time. This difficulty is overcome to some extent by using parallel computations; typically a 500,000 cell problem can be run efficiently on 10 processors in a Linux cluster in one week. NETL researchers recently completed the simulation of the transport gasifier with certain design modifications. As usual, these calculations took around a week to complete. However, the implementation of the design changes in the reactor would take almost a year. NETL researchers already completed the calculations and presented the results at the last PSDF review meeting. The results show a significant increase in CO mole fraction in the exit syngas because of changes in the hydrodynamics inside the reactor. Engineers at PSDF were delighted to see these predictions because the design modifications were specifically made to achieve such high CO mole fractions in the syngas. The calculations have already shown that their expectation would be realized when the modified reactor is operated. Furthermore, construction of the new reactor has recently been completed and the measured syngas concentrations agreed favorably with model predictions made during the construction phase.

The success of the model predictions described above and the ability to conduct simulations prior to the completion of design modifications has successfully moved model predictions to center stage at the PSDF. No longer are model predictions looked at with a high degree of skepticism, rather this model is now considered a valuable tool at PSDF that can be used to provide a variety of information. Engineers at PSDF are using the model to understand the impact the exit has on syngas composition and the effect of reactor height on CO production. They are using the model to understand how the coal enters the reactor and how gas temperature varies inside the reactor. The model has been used to study the effect of increasing the pressure. These high-pressure simulations are being conducted in anticipation of scaling-up the transport reactor to a commercial scale. Recently, Southern Company and others were awarded a U.S. Department of Energy Clean Coal Power Initiative (CCPI) contract to demonstrate transport coal gasification on a commercial scale. Coal gasification at this scale is expected to take place at very high pressure. Design engineers at Southern Company and KBR are using the PSDF simulations conducted at high pressure, parametric studies on the exit configurations, and extending the length of the riser to help in the design process of the CCPI gasifier.

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