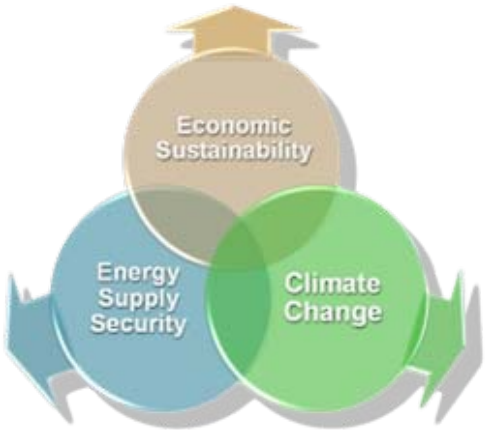
NATIONAL ENERGY TECHNOLOGY LABORATORY



Follow up to 2006 NETL Multiphase Workshop

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Focus Area Leader

Computational and Basic Sciences

2006 Workshop Vision

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 we need integrated research in computations, theory, and experiments!

2006 Workshop Organization

NETL Organizing Committee: *S. Benyahia, R. Breault, A. Cugini, I. Gamwo, C. Guenther, C. Ludlow, M. Massoudi, T. O'Brien, W. Rogers, R. Romanosky, M. Syamlal*

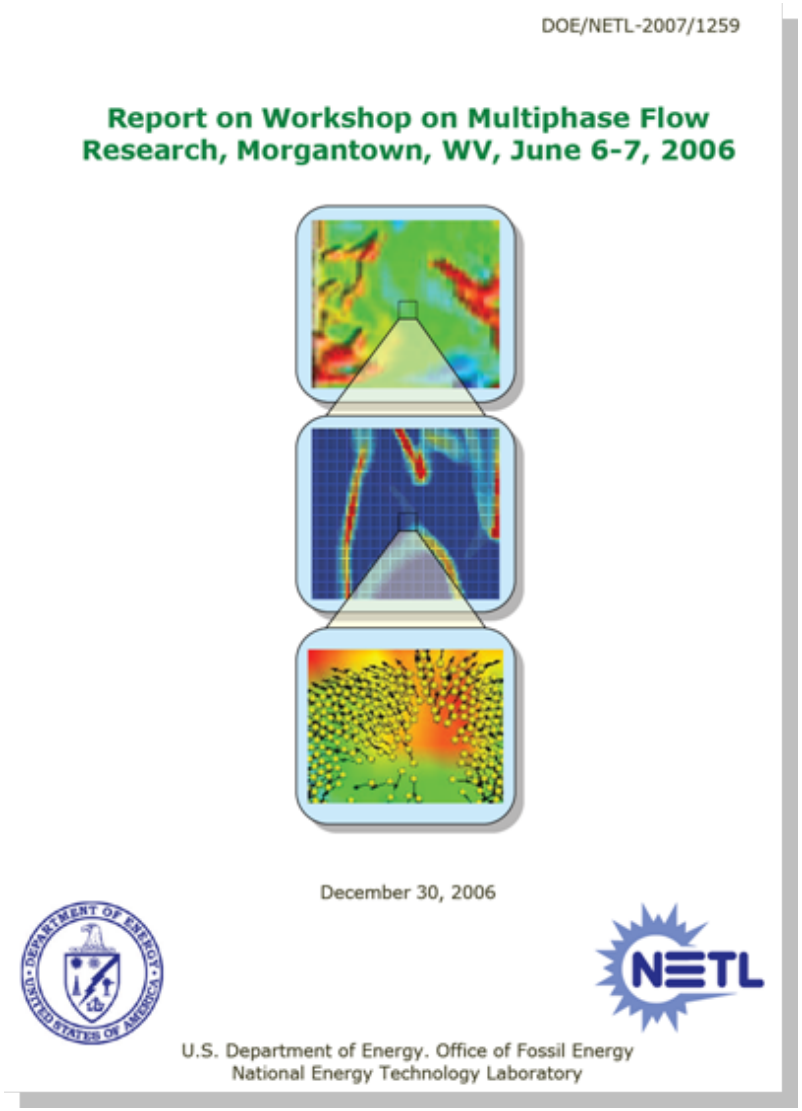
External Advisor: *S. Sundaresan*

TRACK	CHAIR (Industry)	CO-CHAIR (University)	NETL CHAMPION
1. Dense gas-solids flows and granular flows	P. Mort	J. McCarthy	R. Breault
2. Dilute gas-solids flows	R. Patel	S. Subramaniam	S. Benyahia
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*

2006 Workshop Outcome

- Workshop Report
  - ***http://tinyurl.com/c9r7ux***
- Technology Roadmap
  A. Benchmark Cases
  B. Numerical Algorithm and Software Development
  C. Theory and Model Development
  D. Physical and Computational Experiments
  E. Communication, Collaboration, and Education
- Follow up Activities



Extramural Research Supported by NETL (2006-2009)

- **University Coal Research (UCR)**
  - *Texas A&M*: Reduced order modeling
  - *Princeton*: Coarse-graining
  - *IIT*: Mass transfer & dispersion
  - *Princeton, Iowa State, CCNY*: Frictional Flow
  - *Michigan, Florida*: Jet penetration and shape effects
- **Historically Black Colleges and Universities (HBCU)**
  - *Florida International*: Cluster dynamics
  - *Puerto Rico, IIT*: Polydispersed flows
- **Advanced Research**
  - *Colorado, Iowa State, Princeton, PSRI*: Polydispersed flows
  - *Ohio State*: Capacitance Imaging
- **FWP and SSC**
  - *AMES Lab*: DQMOM, DEM, multiphase turbulence, Lagrangian-Eulerian benchmark simulations
  - *ORNL*: ROM, DEM, Square CFB, MFIX parallelization
  - *Pittsburgh, CMU*: Rough annular shear cell experiments and modeling
  - *WVU*: C_3M extension, DEM-Continuum hybrid

In-house Research at NETL (2006-2009)

A. Benchmark
- Validation studies using Barracuda, Fluent, MFIX

B. Algorithm/Software
- Discrete-Continuum hybrid
- Lagrangian-Eulerian
- MFIX-NG, Cartesian grid
- MFIX on 1000's of cores
- Reduced Order Model

C. Theory/Model
- Frictional Flow
- Polydispersity
- Transport Gasifier
- Hydro-gasification
- Chemical Looping System
- CO_2 Capture Devices

D. Physical/Computational Experiments
- Circulating Fluidized Bed Experiments
- High-speed Particle Imaging

E. Communication, Collaboration, and Education
- MFIX OS website
- Chairing IEA's executive committee for the Implementing Agreement on Multiphase Flow Sciences
- Book on Computational Multiphase Flow
- CFB Challenge Problem
- Multiphase Workshop and Powder Tech Special issue

Revisit 2006 Technology Roadmap

- **Wish list from 2006 workshop, guide for future development**
  - Not a project plan; did not define who will do or fund the work
- **NETL has continues to support in-house and extramural research aligned with the roadmap**
- **The roadmap is revisited in the following slides**
  - Work done or supported by NETL are identified
  - ✓ *Research groups engaged in relevant activities identified, doesn't imply that the goals have been met*

A. Benchmark Cases

Near-Term (by 2009)	Mid-Term (by 2012)
1. Hydrodynamics-only simulation of transport reactor to run on 2009 computer cluster overnight 2. ROM for process simulators ✓ Texas A&M, NETL, ORNL	1. Hydrodynamics with heat and mass transfer simulation to run on 2012 computer cluster overnight 2. Repeat Near-Term Case 1 with density variations 3. ROM for process simulators

B. Numerical Algorithm and Software Development – 1

Near-Term (by 2009)	Mid-Term (by 2012)
1. Improve numerical stability and parallel efficiency ✓ NETL, ORNL, WVU 2. Protocol for the integration of various codes 3. Develop coarse-grained (filtered) two-fluid models ✓ Princeton 4. ROM for use by design engineers ✓ NETL, ORNL, Texas A&M	1. Predict transition in the fluidization behavior of Geldart group B to A 2. Fully coupled reactive multiphase flow model ✓ NETL, WVU 3. Automated procedure to coarsen hydrodynamics for use with complex reaction networks ✓ DE-FOA-0000059, due 5/12/09: Multizonal Reduced Order Model Development for Gasification and Combustion Reactors

B. Numerical Algorithm and Software Development – 2

Near-Term (by 2009)	Mid-Term (by 2012)
5. Capture the effect of P, T 6. Document the "current best approach" 7. Identify a standard approach for multiphase flow code verification 8. Validation test cases and computational challenge problems ✓ NETL, PSRI	4. Multiphase ISAT ✓ Iowa State/AMES Lab 5. Explicitly account for the micro/meso/macroscale picture 6. Software framework that allows multiple codes to work together 7. Solve numerical issues with the treatment of PSD (e.g., DQMOM) ✓ Iowa State/AMES Lab

C. Theory and Model Development – 1

Near-Term (by 2009)	Mid-Term (by 2012)
1. Stress and flow fields in dense particulate systems ✓ Princeton, CCNY, Iowa State 2. Drag relations for particle-size/density distribution ✓ Princeton 3. Stress relations for dilute poly-disperse systems ✓ Colorado, Puerto Rico, IIT, NETL 4. Formulate proper boundary conditions	1. Continuum descriptions of dense particulate systems 2. Transition between regimes of enduring contact to collisional contact 3. Model adsorption/desorption and heterogeneous chemical reactions ✓ NETL, WVU 4. Models of electrostatic and van der Waals (cohesive) forces

C. Theory and Model Development – 2

Near-Term (by 2009)	Mid-Term (by 2012)
5. *Understand the cause and effects of particle clustering* ✓ *IIT, Princeton* 6. *Constitutive relations for continuum models from discrete models* ✓ *Iowa State, CCNY, Princeton, Pittsburgh, CMU* 7. *Gas-liquid and gas-liquid-solids flow-regimes and constitutive relations*	5. *Liquid feed injection and subsequent evaporation* 6. *Flow regime transitions in gas-liquid flows* 7. *Radiation model for particle-particle/particle-wall transfer* 8. *Constitutive models for non-spherical particles* ✓ *Florida, Michigan* 9. *Turbulence models with volume fraction fluctuations* 10. *Effect of lubrication forces in particle-particle interactions*

D. Physical/Computational Experiments – 1

Near-Term (by 2009)	Mid-Term (by 2012)
1. Detailed CFB data at two scales (~0.15 m and ~0.6 m diameter vessels) ✓ NETL, PSRI, Florida International 2. Non-intrusive probes for simultaneously measuring the velocities and volume fractions ✓ NETL, PSRI, Michigan, Florida International 3. Experimental techniques for opaque multiphase mixtures	1. Define material properties for use in models and their measurement standards 2. Determine the effect of particle size distribution on flow ✓ Colorado, PSRI 3. Measure spatial variation of PSD 4. Multiphase chemical reactor experiments

D. Physical/Computational Experiments – 2

Near-Term (by 2009)	Mid-Term (by 2012)
4. Measurements of near wall phenomena ✓ NETL 5. Small-scale experiments to provide data to validate sub-models ✓ Pittsburgh, CMU 6. Standardized experiments or simulations (e.g., LBM) to derive custom drag formulas	5. Effect of flow-generated electrostatic forces on dilute gas-solids flows 6. Flow fields in the presence of obstacles (e.g., heat transfer tubes) 7. Measurement techniques for high PT bubble columns 8. Detailed data from 3-D tomography (MRI, X-ray, capacitance imaging etc.) ✓ Ohio State

E. Communication, Collaboration, and Education

Near-Term (by 2009)	Mid-Term (by 2012)
1. Task force to define benchmark gas-liquid and liquid-solids problems 2. Communications network for the multiphase research community ✓ NETL 3. Educational outreach	1. Communication between entities working on OS codes ✓ NETL 2. Challenge problems for multiphase flow with heat & mass transfer and chemical reactions

Discussion Topics

- What do we need to do to accomplish the vision?
- How do we refine the roadmap based on our current understanding of the state-of-the-art?

A. Benchmark Cases

- How do we get benchmark simulations to run overnight on clusters? Is running on 1000's of cores relevant?

B. Numerical Algorithm and Software Development

- BCs for polydisperse continuum simulations
- Multiphysics/multiscale coupling need to be considered

C. Theory and Model Development

- ROM and sub-grid models for reactive, non-isothermal flows

D. Physical and Computational Experiments

- Availability of data from NETL and PSRI risers?
- Computational experiments for model validation (e.g., MD, DEM)?
- Bench-top experiments to test the various phenomena in isolation

E. Communication, Collaboration, and Education

- How to increase collaboration between different research groups? Regular meetings, every year?
- Increasing funding for research in this area, especially for universities

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