Summary of input from participants of Track 2: Dilute gas-solids flows

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Process in Breakout Track 2

- Open forum was used to identify an expanded list of issues not already in opening presentation
- Voted on Pragmatic and Experimental needs: Priority and Term (S/M/L)

NEXT STEPS:

- Paper vote on Fundamental Needs (to be done)
- Summarize workshop findings
- Write Report

List of Participants Who Submitted Input

- **Academic**
  - Goodarz Ahmadi (Clarkson University)
  - Lance Collins (Cornell)
  - Dimitri Gidaspow (IIT)
  - Veeraya Jiradilok (IIT)
  - Donald Koch (Cornell University)
  - Sankaran Sundaresan (Princeton University)
  - Shankar Subramaniam (ISU)
  - Corey O'Hern (Yale University)
  - Narayanan Menon (University of Massachusetts-Amherst)
- **National labs**
  - Sreekanth Pannala (ORNL)
  - Bryan Kashiwa (LANL)
  - Tim O'Hern (SNL)
  - Ron Breault (NETL)
- **Industry**
  - Bing Sun (UOP)
  - Reza Mostofi (UOP)
  - Rutton Patel (ExxonMobil)
  - Sofiane Benyahia (Fluent Inc.)

Input Classified Under 3 Themes

- **Pragmatic Needs**
  - For ongoing modeling applications
  - CFD in extensive use by industry and improvements are needed near term
- **Experimental Needs**
  - Crucial to tie models to well defined experiments
- **Fundamental Needs**
  - For major improvements with well grounded theory
  - Replace pragmatic approach as better models developed

Pragmatic Needs

- **Drag law applicable over entire range of solids fraction High, 3 Y**
  - Dilute flows include locally dense regions – e.g. at entrance and walls
  - Fluid-particle force at particle scale (effect of neighbor particles). DNS to ascertain these effects at particle scale.
- **Coarse graining (filtering) of two-fluid models High, 3 Y**
- **Role of gas-phase turbulence - importance for gas-solids flows ... Pragmatically can we neglect? Low 10Y**
- **Models and constitutive relations to handle particle size distribution (psd) High, 5Y**
  - Computational framework with speed of computation
  - Validated constitutive models
  - Multi-particle kinetic theories
  - Two-fluid EE models for particle deposition and re-suspension, effect of psd
- **Models for non-spherical particles in non-dilute flows ... LB methods? Medium, 5Y**
  - Reactivity (not important, (Niksa)
  - Collisional important for dense flows (Jennifer)
- **Two-way interaction models of two-equation or stress transport type for Lagrangian-Eulerian and EE models for gas-solid flows with heat (and mass) transfer (Deferred)**

New list

- **Particle dispersion in fuel injectors and gasifiers. (Niksa).**
  - Particle dispersion is part of the hydrodynamics computed from Re stress (Dimitri, Chem. Eng. Science paper 2006) comment
  - Important to simultaneously capture particle dispersion and fluctuating KE in both phases simultaneously (Shankar) Fund
  - PSD and shape (Malhotra, Niksa) All
- **Effect of temperature and pressure (Wen Chen). Validation of models of transition of B/A (fundamental, there are data, Wen Chen)**
- **Effect of particle attrition and agglomeration. 1M lb → 30 lb per hour (sand). For coal is meant fragmentation (Niksa). Experimental input (relatively easy Wen Chen) to Pragmatic solution**
- **Particles (coal) generate gas, which affect the fluid dynamics (Liu). Fundamental and Pragmatic**
- **Heterogenous chemical reactions, adsorption/Desorption (Ray).**
  - CFD not suited for handling complex (stiff) reactions. Equivalent reactor network extracted from CFD (Niksa, Patel). Pragmatic
  - Other methods as ISAT (Shankar) can be used with full CFD simulation. Fund
- **Liquid injection and evaporation (Ray) All**
- **Radiation from wall and particles (?) (Ray, Niksa) Fund & Prag (walls)**
- **Electrostatics to investigate at least in cold flow (Tim) Prag and Exp (George, empirical corr.) Fund (Ahmadi). Charge to mass ratio issue (Dimitri). Van Der Walls (cohesive) forces (Ahmadi).**
- **Particle deposition & Re-suspension in dilute flows (Niksa) Prag**
- **Internals (obstacle, heat transfer tubes, etc.) (Wen Chen) Exp & Prag (quantitative comparison)**
- **Erosion (Bill – exp data at NETL, Patel) Prag & Exp (Ahmadi model and exp from Oklahoma, Shirazi ?)**

Pragmatic Needs (2)

- **Particle collision Low 5Y**
  - Effect on momentum, heat and mass transfer during particle collision
  - Angular momentum transfer for rough particles (Tom)

- **Fully coupled reactive flow model High 10-15Y**

- **Industrial scale reactor computations High 3-15Y**
  - How to handle relatively large size cells … granular temperature equation less relevant?
  - Single cluster size approach – alternatives?
  - Fast reduced order models from accurate computational results to be used by design engineers

NETL

Experimental Needs

- **Long term program - multiple years - to provide detailed data on at least 2 scales (~0.15 m and ~0.6 m) High 3Y**
  - Well characterized – entrance, exit, boundaries
  - Local pressure, velocity of solids and gas, solids fraction, fluctuations, …
  - Cluster size
  - Solids flux – resolve measurement method

- **Specific test for each phenomena in conjunction with input from modelers Medium 5Y**
  - Gas/solids drag, measure both gas and solids velocities (slip) (Wen Chen and Dimitri).
  - Full numerical (DNS + DEM) Fundamental

- **Effect of entrance geometry and preconditioning**

- **Calibrated diagnostics – non-intrusive**
  - Simultaneous gas and solid phase measurement
  - Planar flow field rather than point-to-point traverses
    - E. g. Radial solids concentration in riser by MRI
    - Solids, gas velocities and turbulence using combination of PIV and laser sheet (applicable to very dilute flows)
  - 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%) to take into account:
    - Frictional interactions
    - Bidisperse or polydisperse grains
    - non-spherical grains

Experimental Needs (2)

- **Near wall measurements**
- **Effect of psd**
  - Binary mixture – lateral distribution of particle types, segregation
  - Continuous psd – measure spatial variation of psd
- **Measure characteristic parameters used in models – fine scale**
  - Collisional parameters, internal angle of friction, etc.
- **Detailed measurements in reactive flow with simple chemical reaction, e.g. ozone decomposition**

Fundamental Needs

- **Particle Clustering**
  - Understanding of physics, instability leading to fluctuations in concentration, scaling with parameters
  - Predictive model for preferential concentration of particles in turbulence
  - Effect of particle clustering on drag, collisions, turbulence modulation
- **Effect of electrostatic and particle surface forces**
  - Is electrostatics unimportant at process temperatures?
- **Filtering procedures to rigorously extend LES to multiphase flows**
  - Valid over a broad range of parameters: light to heavy particles, all size ranges
  - Sub-grid scale models with correct physics
  - LES to tackle effects of clusters and inhomogeneous distributions
- **Modeling multiscale interactions**
  - How particle clustering affects fluid flow structure at different scales
  - Interaction of a particle with turbulent eddies of different length and time scales.

Fundamental Needs (2)

- **Development of kinetic theory based on qualitative and quantitative input from:**
  - Soft sphere simulations (already available)
  - 3-D collisional model for rigid, inelastic, frictional particles

- **Theoretical challenges in mathematical formulations of multiphase flow**
  - Satisfactory resolution of ill-posedness of EE multifluid equations
  - Eliminate the need to time-average EE two-fluid solutions for statistically steady problems
  - What level of mathematical representation is needed in both EE and LE approaches to capture physical phenomena
  - Rigorous measure-theoretic re-formulation of the Eulerian-Eulerian EE multifluid approach
  - Consistently incorporate fluctuations in the volume fraction
  - Consistency conditions between EE and LE models, especially for correlations in particle-laden turbulent flow
- **Boundary conditions High 3-5Y**
  - Treatment of exits
  - Wall boundary conditions – do they capture key effects? e.g. shape of solids flux distribution near wall
  - Use DEM