A) Modeling: existing approaches, confidence in these approaches, validation of these models, and future prospects for improving existing models.

- Continuum two-fluid descriptions. Work well mostly for group B and D particles but have problems when transitions from dilute to dense flows. I think a more comprehensive theory is needed to model the granular phase all the way from dilute to dense regimes.
- DES coupled with flow solver. Very expensive to use currently on any realistic systems. Statistical sampling techniques to down-size the number of particles would be very useful and at the same time parallel modules have to developed so that it is easy to port DES-Flow solvers easily for good parallel efficiency on large-scale High Performance Computing (HPC) platforms.
- One area which is relatively at the inception is the hybrid DES and continuum simulations. We term it as DECM (Discrete Element Continuum Model). This model has to be generalized so that only particular particle size or particular region (geometrically or in some variable space) of the domain can be solved by DEM while rest can be solved using the continuum model. This has tremendous promise but the framework currently needs too many heuristics. The other subtopic within this approach is to have in-situ DEM calculations to derive stresses etc. for the continuum simulations.
- In fluidized bed reactors there is still lot of uncertainty in the correlations employed for heat- and mass-transfer as well as heterogeneous chemical reacting flows. Better correlations are needed and one can trend started by detailed Lattice-Boltzmann simulations employed to improve drag correlations by employing new multiscale techniques to model flow around the particles along with heat- & mass-transfer and chemical reactions.

B) Experiments: what well-defined experiments exist, what experiments are needed, and

- Need well defined benchtop experiments to easily characterize parameters which go into numerical simulations (like average coefficient of restitution, internal angle of friction etc.)
- Need benchtop experiments (similar to bin-discharge) which can be used to study cluster formations.

C) Design needs: what information do design engineers need, and how much of this information is currently available from models and experiments.

- Design engineers need fast real-time models which can be used for parametric runs or for actual implementation in model based controls. We need to establish well-defined procedures to arrive at reduced order models from the computational data of Hi-Fidelity models.

Modeling and simulation challenges and approaches to address these challenges for:

1) Immediate (next 3 years),

- Looking at dense-to-dilute transitions and make engineering improvements.

- Validation and verification of continuum models for large scale systems. Identifying error bars in the current state-of-the-art simulations and the sources of these errors to guide future development.
- Multiscale modeling of the surface processes along with the near particle flow field effects.
- Hybrid DEM-Continuum formulations.

2) Medium Term (next 3-6 years) and

- Extend the multiscale modeling from atomistic scale to device scale.
- Writing scalable software for multiphase flows which can utilize 10s of thousands of processors very efficiently.
- Rigorous procedures based on detailed computational data or new algorithmic developments to reduce the dimensionality of the fluidized bed reactor problems and arrive at reduced order models.

3) Long-term (6-9 years)

- Employ both continuum and hybrid models to accurately model industrial scale devices and aid in design and optimization of the devices.