Toward understanding micro-macro relations of solids flow with an eye on process performance
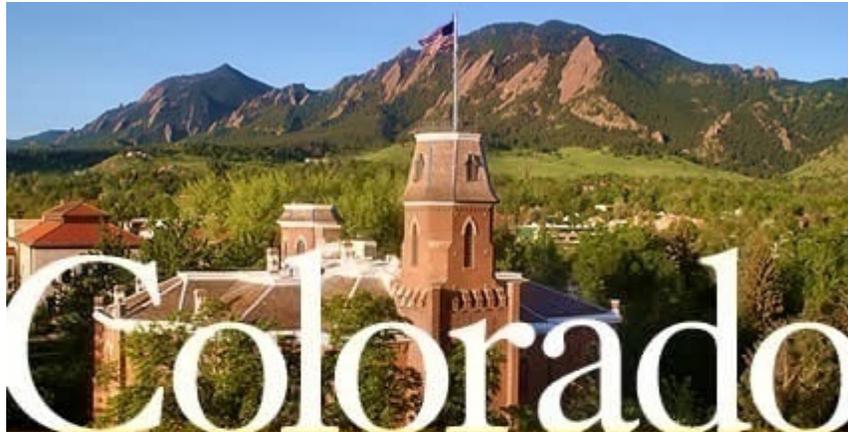

Christine Hrenya

University of Colorado
Chemical & Biological Engineering

IFPRI Powder Flow Workshop
Amsterdam, The Netherlands
January 2017

The charge from the organizers…

"**The syndicate sessions have been framed around three questions:**

    (1)   Characterize the state-of-the-art in powder flow

    (2)   Confront the "grand challenge" to relate particle properties, microstructure, and bulk flow behavior

    (3)   Define three scientific questions that IFPRI and other funding sources should promote

In this context, we hope that your talk will address the 'big picture' suggested by these three questions."
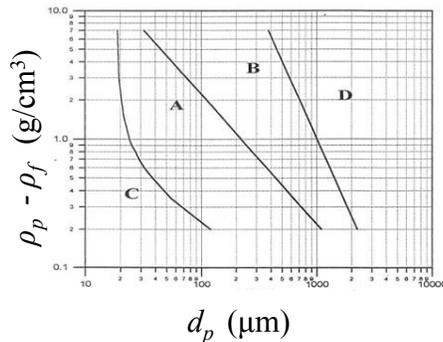
Approach: Discuss in terms of "case study" – cohesive-particle flow project

State of the Art

General comments

- today: rely too heavily on experience, correlations
- goal: accurate prediction of large-scale devices

Case study: Cohesive-particle flows (applicable to other phenomena)

d_p (μm)

Geldart's classification (1973)

- dimensional quantities ⇒ *not universal*
  - -van der Waals
  - -atmospheric T/P
  - -fluidized beds

### Correlations for Entrainment Rates (2015)

- *orders of magnitude differences* between various correlations

Lines refer correlations in literature: 1955 - 2005

Chew, Hrenya, Cocco & Kerri (Chem. Eng. J, 2015)

Normalized gas velocity

Predicting Agglomerate Size (2012)

- *order of magnitude difference* between various correlations

(*Shabanian, Jafari, & Chaouki, 2012*)

In-house shadowgraphy: 49 um particles in fluidized bed riser
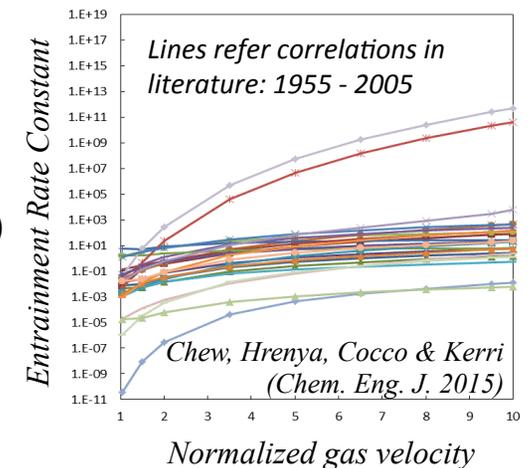
Grand Challenge

"MACRO-SCALE BEHAVIOR BASED ON MICRO-SCALE PROPERTIES"

Step 1: Microscopic Understanding

Step 2: Micro-macro Link

Step 3: Macroscopic Predictions

Grand Challenge

"MACRO-SCALE BEHAVIOR BASED ON MICRO-SCALE PROPERTIES"

Step 1: Microscopic Understanding

- today: *assumed* particle-particle (DEM-type) models and inputs
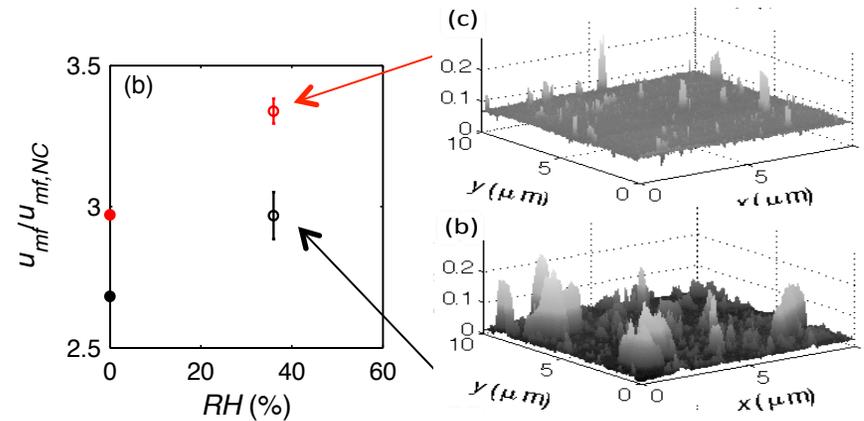- goal: *validated* models

Step 2: Micro-macro Link

Step 3: Macroscopic Predictions

*Q1: Do we have a **validated** microscopic understanding of phenomenon of interest (cohesion, non-spherical particles, etc.)?*
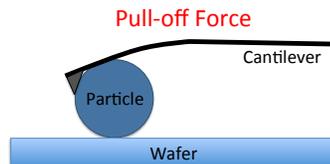
Key elements

- Inputs
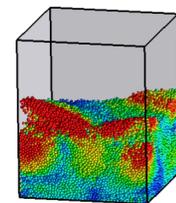 - Experimental particle prop's & ambient conditions often omitted

- Outputs/Validation
  - Micro-level (particle-particle)

    LaMarche, Leadley, Liu, Kellogg & Hrenya (Chem. Eng. Sci. 2017)

    » difficult for complex particle (e.g., non-spherical)

  - Macro-level (many-particle systems)
    » System-size independent measurement

    Liu, LaMarche, Kellogg, Leadlley & Hrenya (AIChE J. 2016)

$N_p \sim 10^7$ $N_p \sim 10^{10}$

Grand Challenge

"MACRO-SCALE BEHAVIOR BASED ON MICRO-SCALE PROPERTIES"

Step 1: Microscopic Understanding
- today: *assumed* particle-particle (DEM-type) models
- goal: *validated* models

Step 2: Micro-macro Link
- today: sensitivity analysis of *specific macro system* to *assumed micro model*
- goal: seek *universal and robust* micro-macro relationships (key physics)
  - Universal = dimensionless
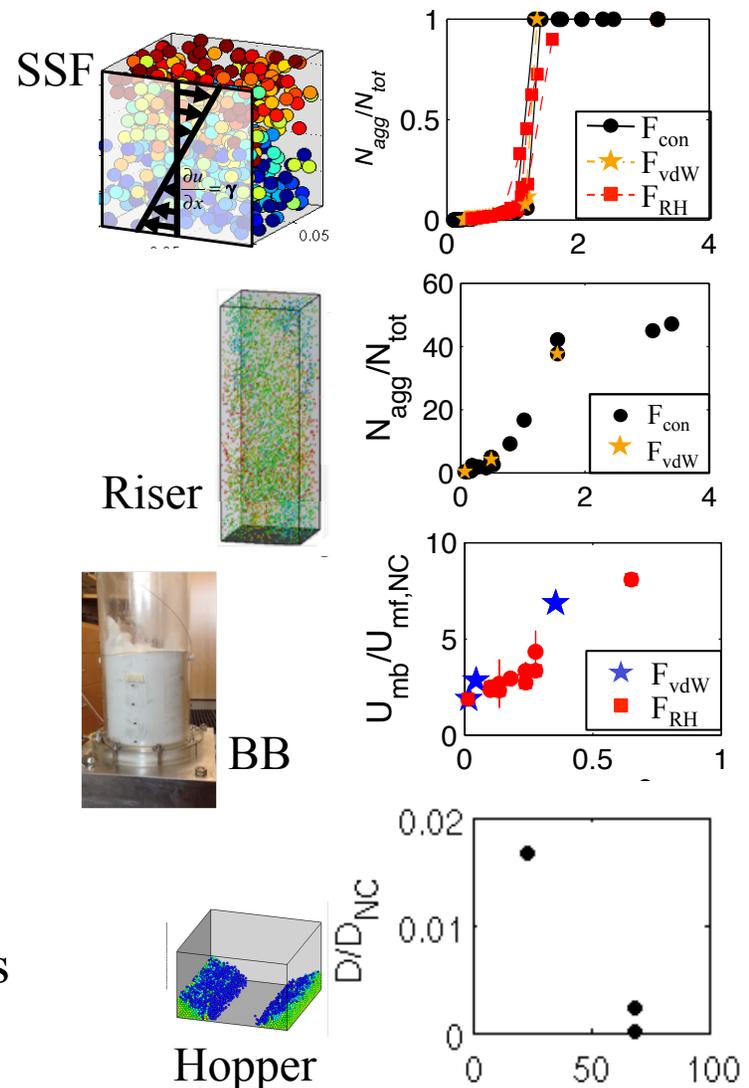 - Robust = applicable to wide variety of systems

Step 3: Macroscopic Predictions

*Q2: Do we have a **universal** and **robust** understanding of the micro-macro link?*

Key elements

- Step 1: Non-dimensional groups
  - Robust (type of cohesion, system, etc.)
  - Key physics
    - » *relevant* microscopic quantities (roughness, force, energy?)
    - » measurement techniques (AFM vs. macro?)

- Step 2: Use validated *micro* models to drive development of *macro* models
  - e.g., population balance

SSF

Riser

BB

Hopper

Grand Challenge

"MACRO-SCALE BEHAVIOR BASED ON MICRO-SCALE PROPERTIES"

Step 1: Microscopic Understanding
- today: *assumed* particle-particle (DEM-type) models
- goal: *validated* models

Step 2: Micro-macro Link
- today: sensitivity analysis of *specific macro system* to *assumed micro model*
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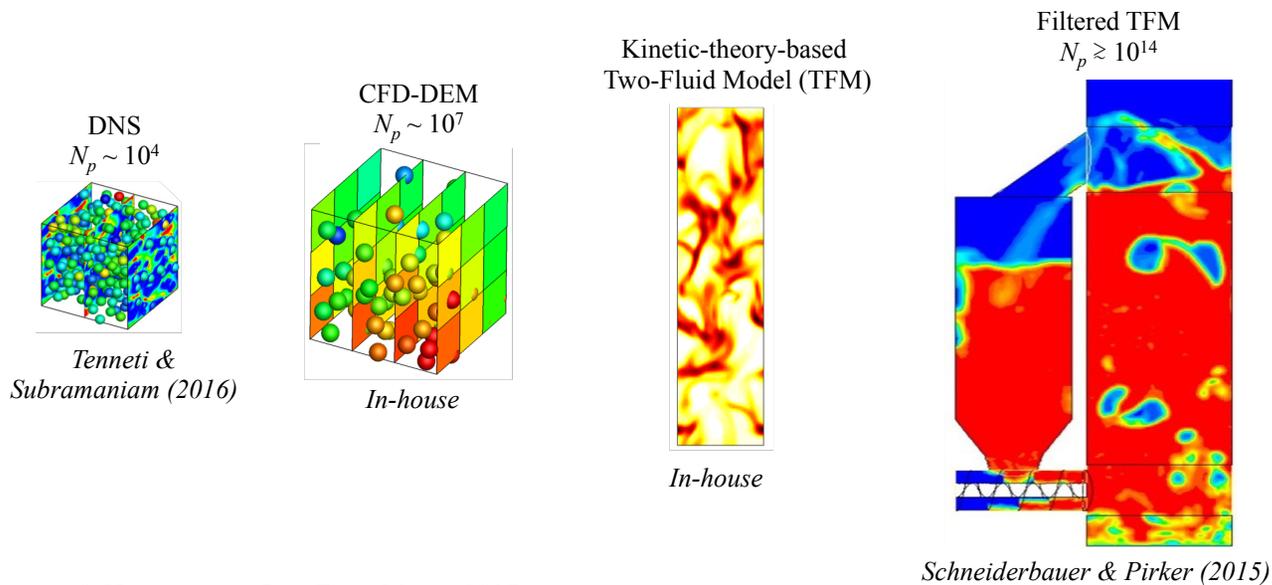
Step 3: Macroscopic Predictions
- today: predict behavior of *small-scale* systems and extrapolate to industrial systems (mostly *qualitative*)
- goal: seek *accurate, quantitative* predictions of *industrial-scale* units

Scientific Question #3: Macro

Q3: Can we perform accurate, quantitative predictions of industrial units?

- Key elements
  - Modeling advancements (DNS, DEM, continuum, filtered, hybrid):
    incorporate micro-level understanding to macro-level models
  - Computational advancements (collaboration with HPC scientists)
  - Transportable to commercial code (technology transfer)

DNS
$N_p \sim 10^4$

Tenneti &
Subramaniam (2016)

CFD-DEM
$N_p \sim 10^7$

In-house

Kinetic-theory-based
Two-Fluid Model (TFM)

In-house

Filtered TFM
$N_p \gtrsim 10^{14}$

Schneiderbauer & Pirker (2015)

Fullmer & Hrenya (Ann. Rev. Fluid Mech., 2017)

(data-driven closures and physical insight)

Industrial funding – lessons learned & key elements

- Significant financial backing for significant period of time
    - Ability to pursue expt/DEM/continuum simultaneously
    - Flexibility to change directions with preliminary results
    - Project is prioritized
- Work on all parts for given phenomenon: micro, micro-macro, macro
- True collaboration between academia and industry
    - Keeps each other focused and builds "team" effort, open communication, vested in each other's success
    - Same is true for academic collaborations – productive collaborations based on papers etc. may be different than accomplishing big-picture scientific goals
- Focus on science and not reporting
    - Monthly .ppt updates rather than reports
- Ability to publish
    - Contract set up such that experiments/simulations done on both proprietary and non-proprietary materials – good for both since publications are essentially required for academics/trainees, and industry does not want to give up any secrets. Does not take up significant extra time since most time is spent building models/experiments, and less on running them