

# Selection of Flow Aids: Model-based Prediction of Flow Properties Enhancements

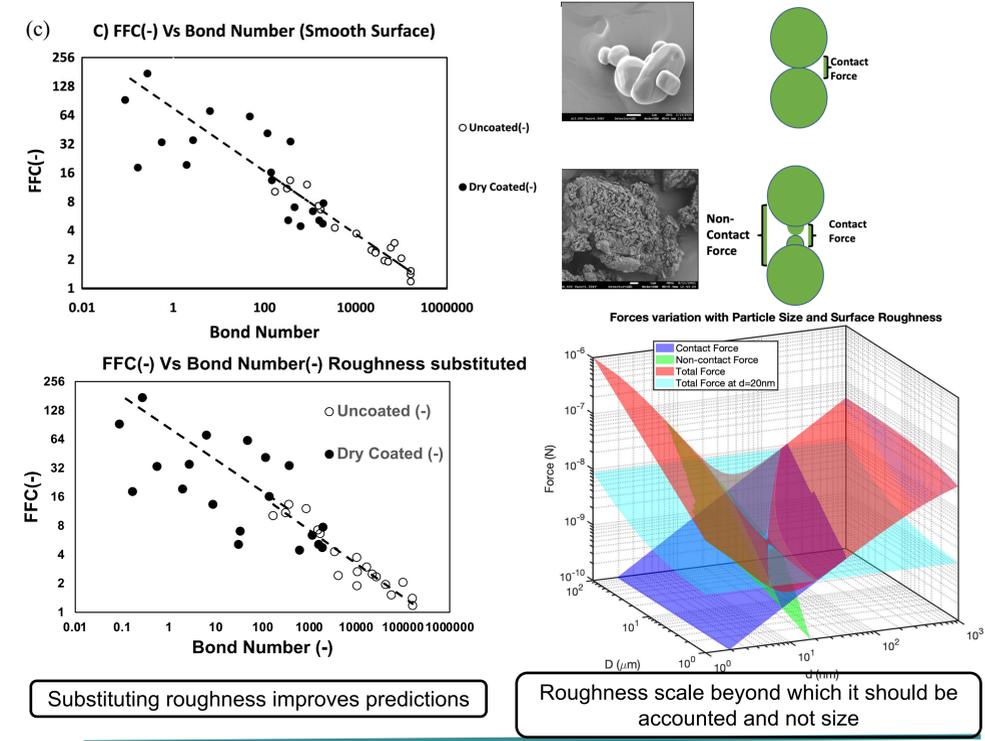
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**Objective:** Mechanistic prediction of flow properties and its enhancements from particle scale measures, developing a collection of models and decision tools that can be used for flow aid selection while minimizing the extent of experiments needed.

**Recent Results:** Significant progress for powder flow enhancements using two types of flow-aids; demonstrated the applicability of models in determining the suitable amount and type of flow-aid; improved contact models for macro-rough surfaces, proposed dry coating guidelines for coating fines vs coarse component in a blend. The analysis of multiple blends revealed positive synergy and enhanced flowability when one component was dry coated. The flow aid performance was examined by dry coating four fine powders with four different flow aids, and the outcomes were explained through integration of different models. The findings underscore that only part of a powder sample needs dry coating, which is a major practical outcome.

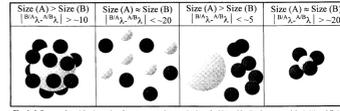
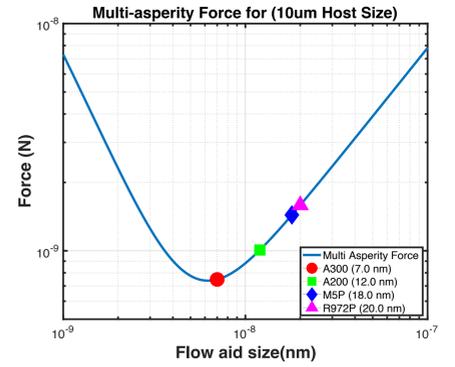
## Mechanistic approach for flow aid processibility



## Model based prediction of flow aid performance

Size based guidance suggesting finest should be the best

Flow Aid	Size (d <sub>50</sub> , μm)
R972P	0.018
M5P	0.020
A200	0.012
A300	0.007

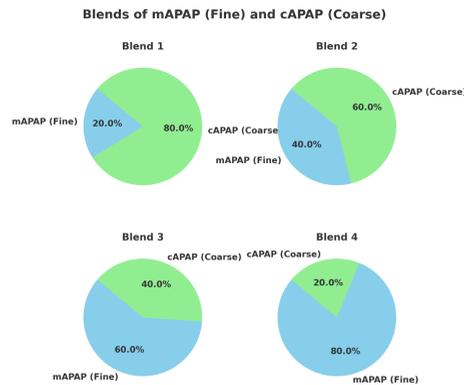
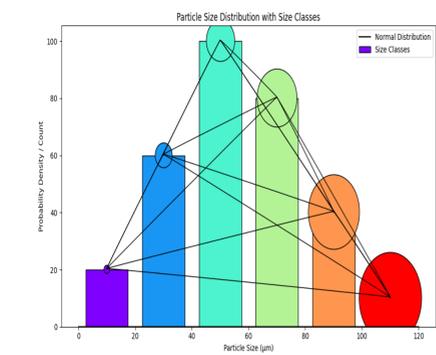
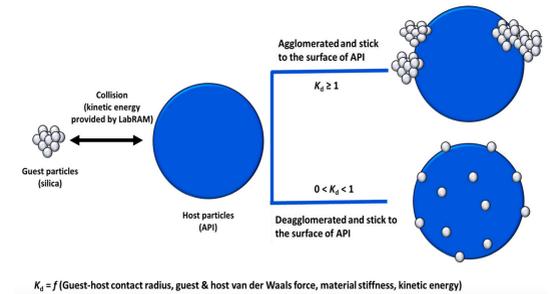


$$B/A \lambda = 4 \left[ \frac{A \gamma_d^B \gamma_p^B}{A \gamma_d + B \gamma_p} + \frac{A \gamma_p^B \gamma_p^B}{A \gamma_p + B \gamma_p} - \frac{B \gamma}{2} \right] \left| \frac{B}{A} \lambda - \frac{A}{B} \lambda \right| = 2 \left| A \gamma - B \gamma \right|$$

Surface Energy Based guest-host compatibility suggesting A300 not as good as R972P

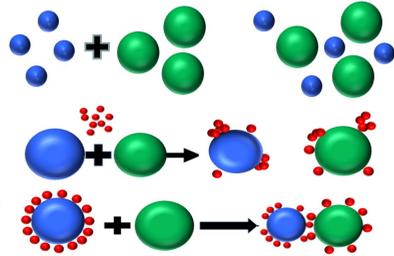
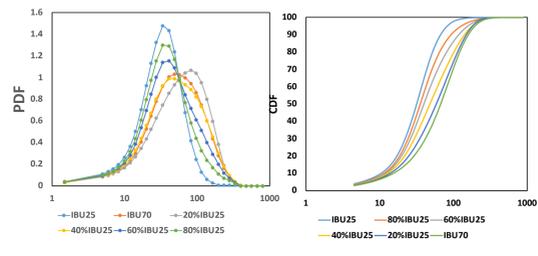
Coated (R972P)	Coated (M5P)	Coated (A200)	Coated (A300)
22.1	3.5	3.0	2.3
30.0	4.4	4.9	10.2

Stick-bounce model → Spreading of flow aid based on intensity and material properties of host and guest



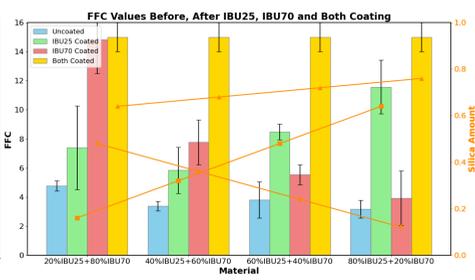
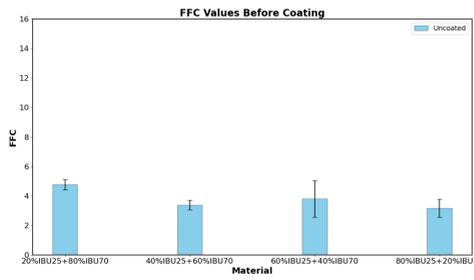
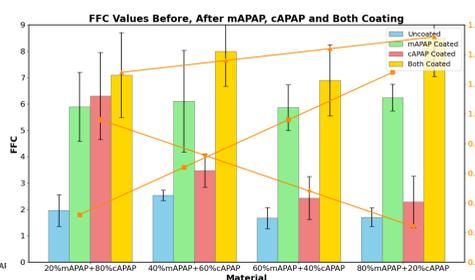
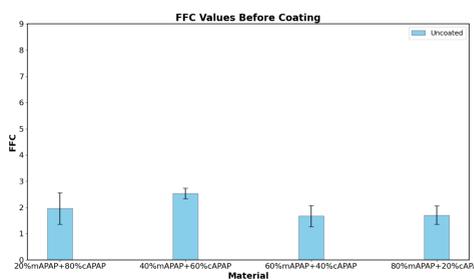
Effect of interparticle interactions with different size distributions

Blends having different wt% of coarse and finer components of same material



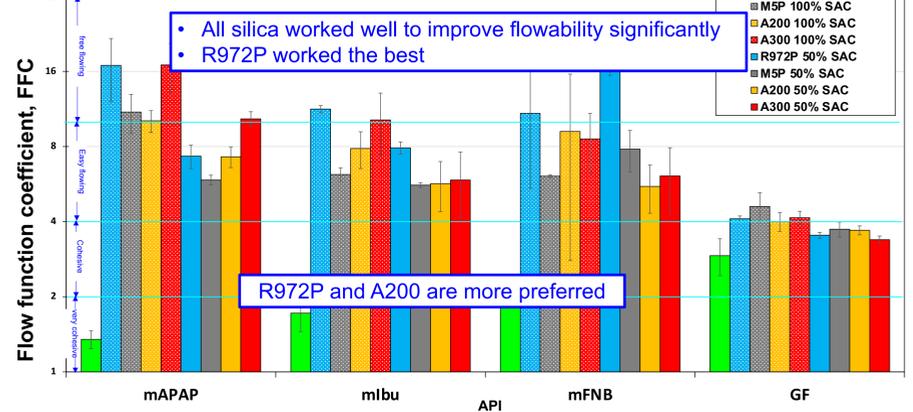
PSD with varied wt.% of fine and coarse components

Possibility of flow aid coating and distribution

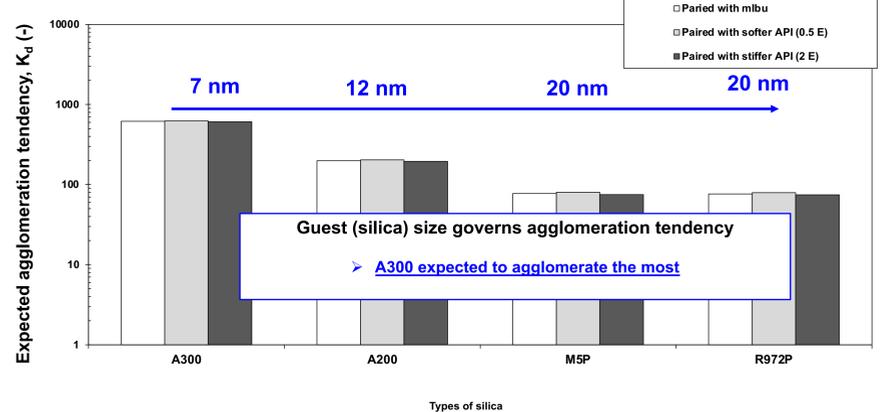


Mechanistic rules guiding coating selection and synergy when a component is coated

## Flowability of API with and without the dry coating



## Expected agglomeration tendency of silica



## Key Learnings

- (1) The contact models work well for coated/uncoated and even non-spherical particles,
- (2) Effect of size distribution captured using cohesion averaging
- (3) Only a small fraction of the powder needs dry coating, and
- (4) Flow-aid performance is best explained through multiple models guiding amount and type of flow aid

## Future Work

- (1) Improving mechanistic models to account for host and guest particle assumptions of smooth host and monolayer uniform coating,
- (2) Developing an integrated simulation package, as well as focusing on industry-relevant experimental topics like effect of processing device parameters, humidity effects, and coating stability



Member input and collaborations are welcome!