IFPRI Project #130

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

Raj Davé
Students: Siddharth Tripathi and Sangah Kim
New Jersey Institute of Technology
May 2024

Outline

- Progress Since Last Year

- Overall Project Achievements and Learnings

- Future directions

Progress since last year

Flow enhancements of ~30 powders; used two different flow-aids

Improved contact model accounting for macro-rough surfaces, addressing outliers

Dry coating guidelines: tools to determine flow-aid amount and type; entire powder sample need not be coated
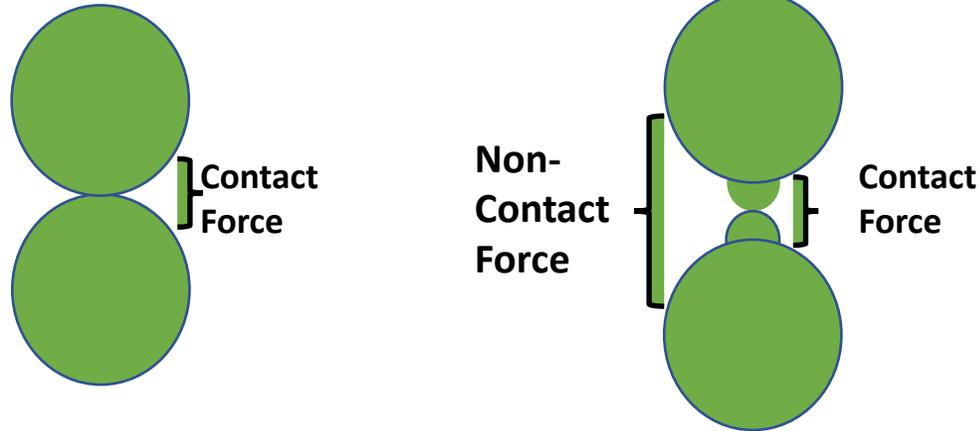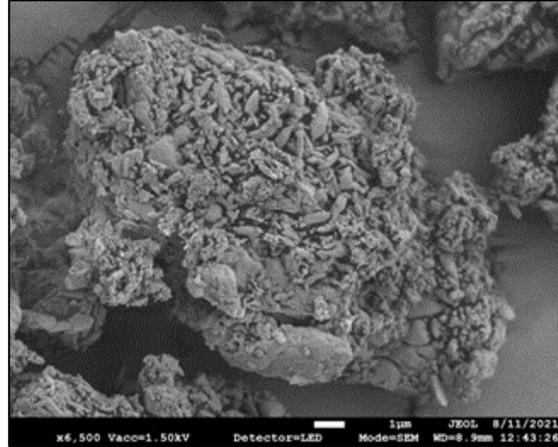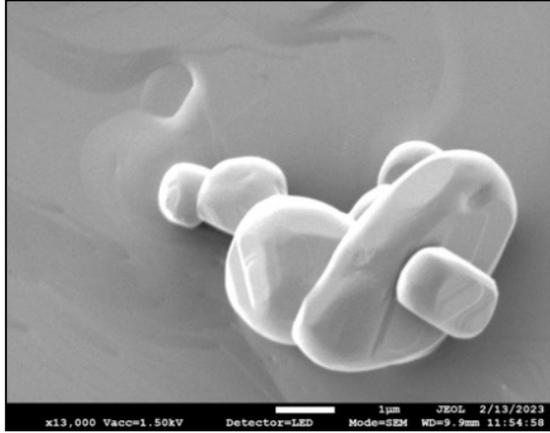
Blending Synergy:
- Analyzed 42 blends where one component was dry coated
- Observed positive synergy of flow enhancement for most blends
- Flowability of mixtures was greater than individual components

Flow aid performance: Four fine powders dry coated with four different flow-aids (silicas)
- Explaining flow enhancement outcomes using integrated models

Contact model accounting for roughness

Contact Force

Non-Contact Force

Contact Force

Forces variation with Particle Size and Surface Roughness

- Non-contact Force
- Contact Force
- Total Force
- Total Force at d=20nm

Total force=Contact + non-contact Force

Contact and noncontact forces depend
on the dimension of roughness
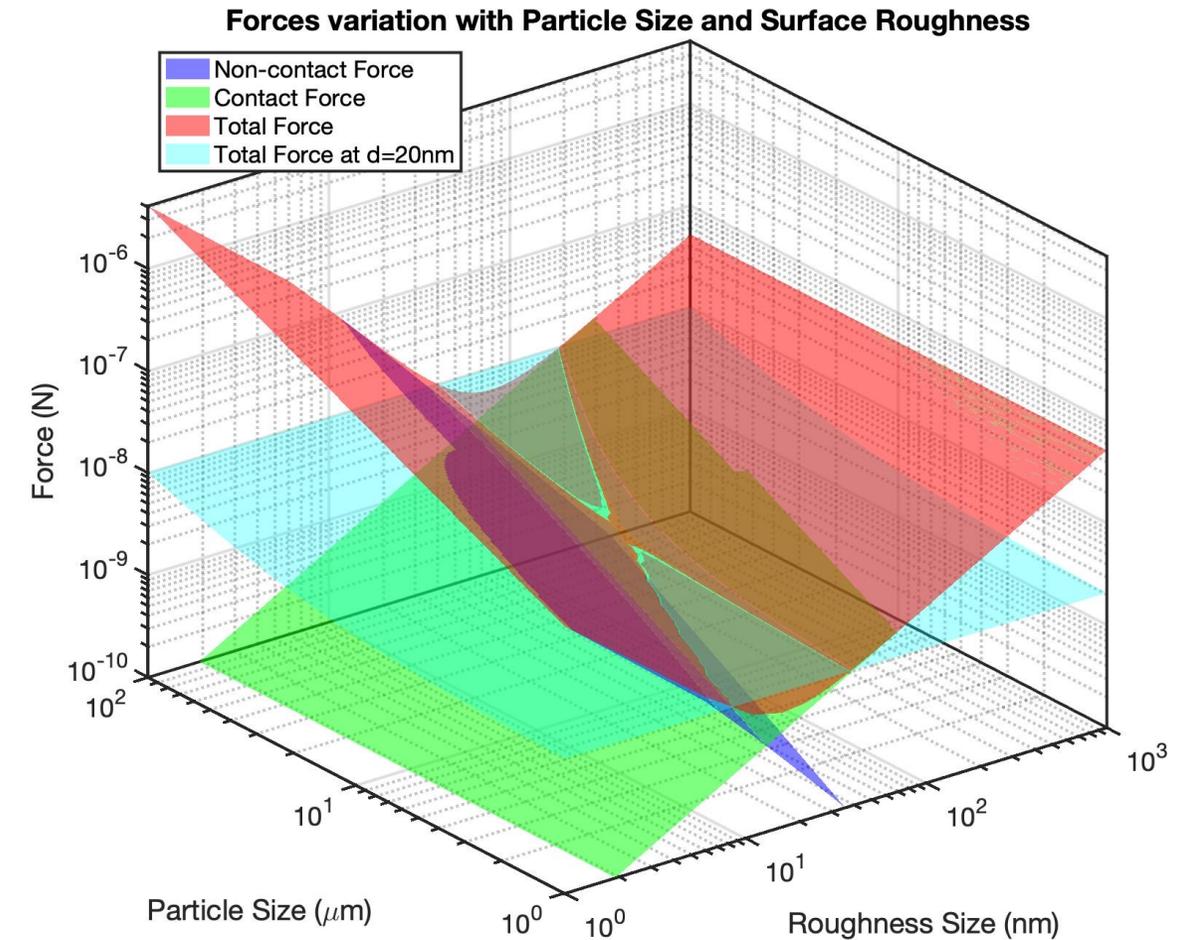
- Particle Roughness dominates in interactions beyond a certain roughness scale.
- Spatial distribution of roughness also matters

Rough particles have less cohesion before dry coating
and the enhancement may be lesser unless more silica is used

Mixing synergy: Silica transfer

Results in synergistic property improvements
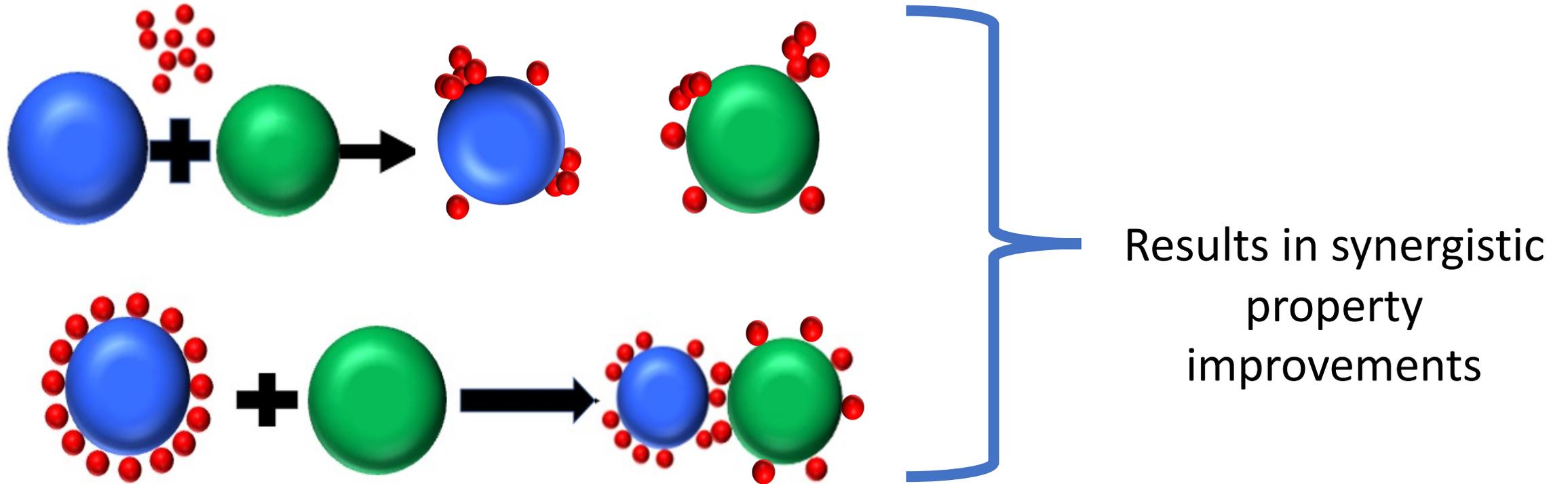
FFC For Uncoated Blends

FFC for Dry coated API (1wt% silica)
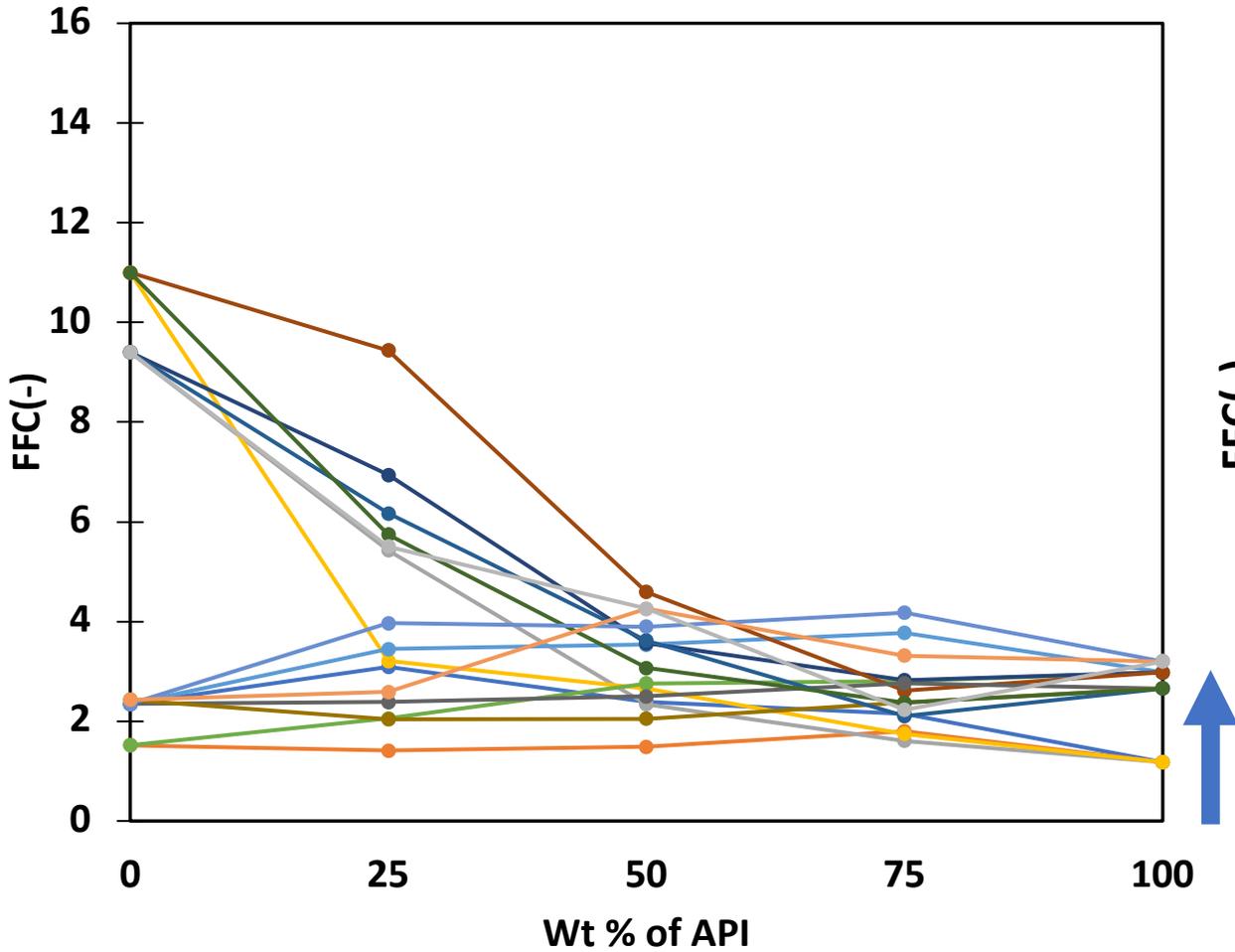
None of the components are coated prior to mixing
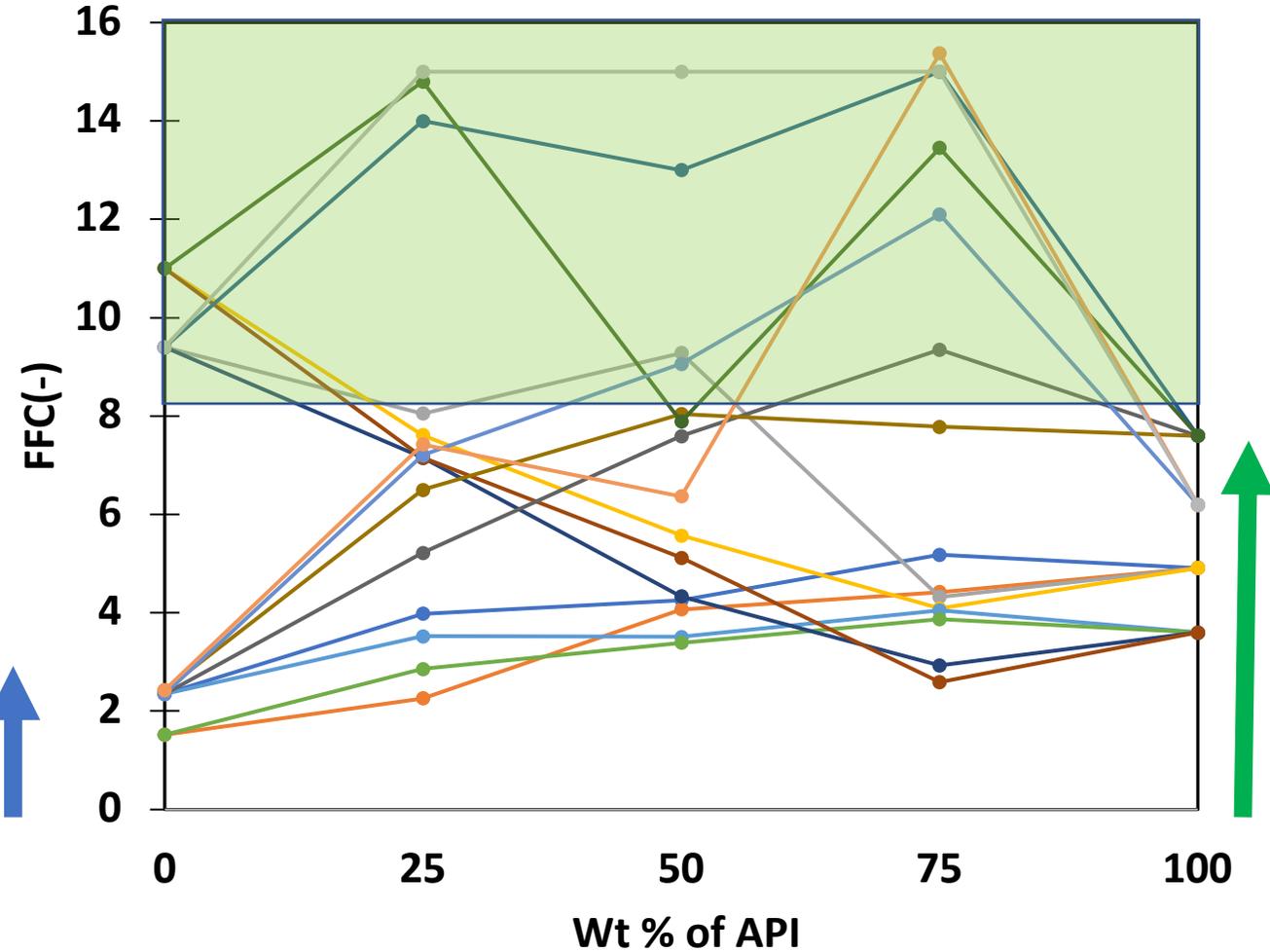
The API was dry coated prior to mixing

Non-linearity and synergies where the resulting bulk property is higher than individual components

13

Selection of Nano Flow Aid: Model-based guidance

Multi-asperity Force for (10um Host Size)

Force (N) vs Flow aid size(nm)

Legend:
- Multi Asperity Force
- A300 (7.0 nm)
- A200 (12.0 nm)
- M5P (18.0 nm)
- R972P (20.0 nm)

Model-based Guidelines:

1. Chen's multi-asperity model ➜ _Cohesion reduction as function of flow aid size_

2. Guest-host compatibility model ➜ Adherence of flow aid based on surface energy difference– not so valid for higher intensity processing

3. Stick-bounce model (Zheng et al. 2020) ➜ Spreading of flow aid based on intensity and material properties of host and guest
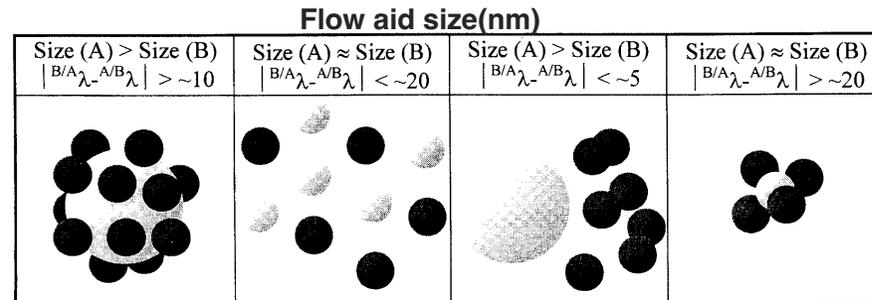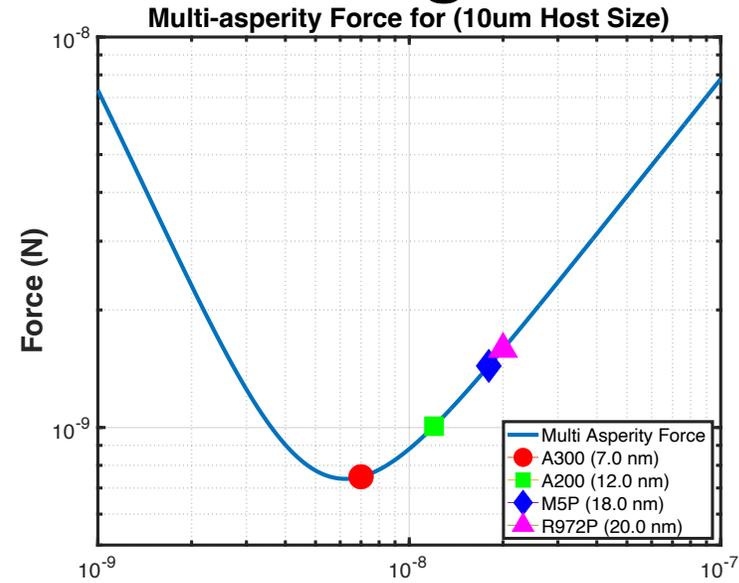
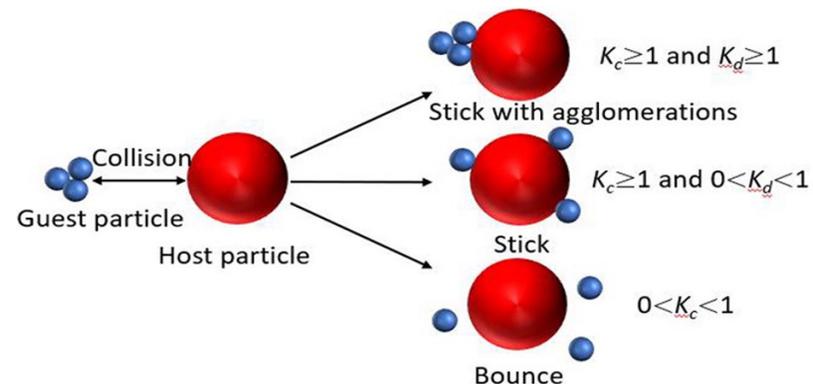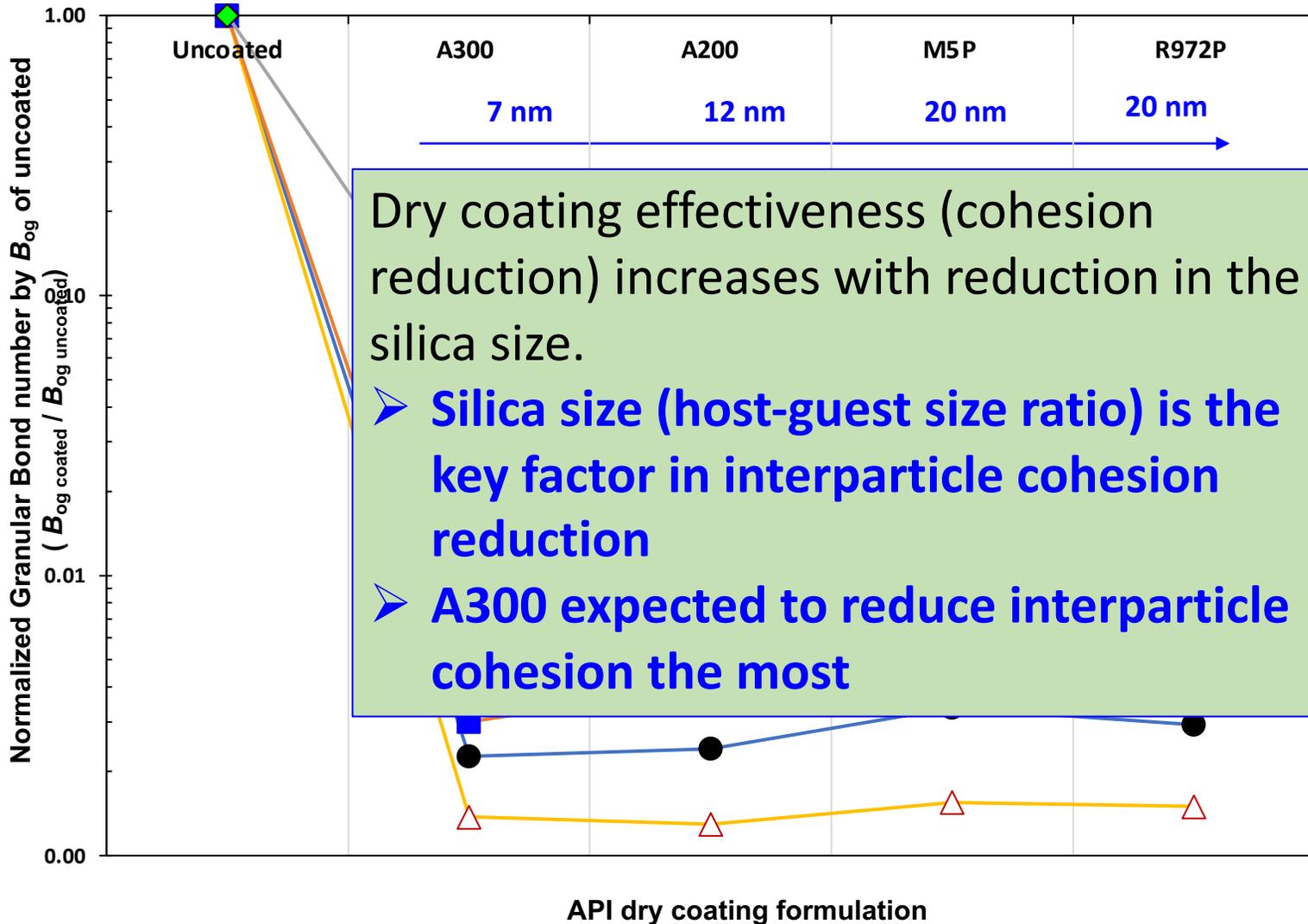| Size (A) > Size (B) $\left| {}^{B/A}\lambda - {}^{A/B}\lambda \right| > {\sim}10$	Size (A) ≈ Size (B) $\left| {}^{B/A}\lambda - {}^{A/B}\lambda \right| < {\sim}20$	Size (A) > Size (B) $\left| {}^{B/A}\lambda - {}^{A/B}\lambda \right| < {\sim}5$	Size (A) ≈ Size (B) $\left| {}^{B/A}\lambda - {}^{A/B}\lambda \right| > {\sim}20$

Fig. 6. Influence of particle size and surface energy on the organisation of a binary blends of two materials A (○) and B (●).

Collision
Guest particle
Host particle

$K_c \geq 1$ and $K_d \geq 1$
Stick with agglomerations

$K_c \geq 1$ and $0 < K_d < 1$
Stick

$0 < K_c < 1$
Bounce

Applying Chen multi-asperity model

Chen model prediction based Bo_g : 50%SAC cases

Normalized Granular Bond number by Bo_g of uncoated ($Bo_{g\ coated}$ / $Bo_{g\ uncoated}$)

Uncoated	A300	A200	M5P	R972P
	7 nm	12 nm	20 nm	20 nm

API dry coating formulation

Dry coating effectiveness (cohesion reduction) increases with reduction in the silica size.

➢ **Silica size (host-guest size ratio) is the key factor in interparticle cohesion reduction**

➢ **A300 expected to reduce interparticle cohesion the most**
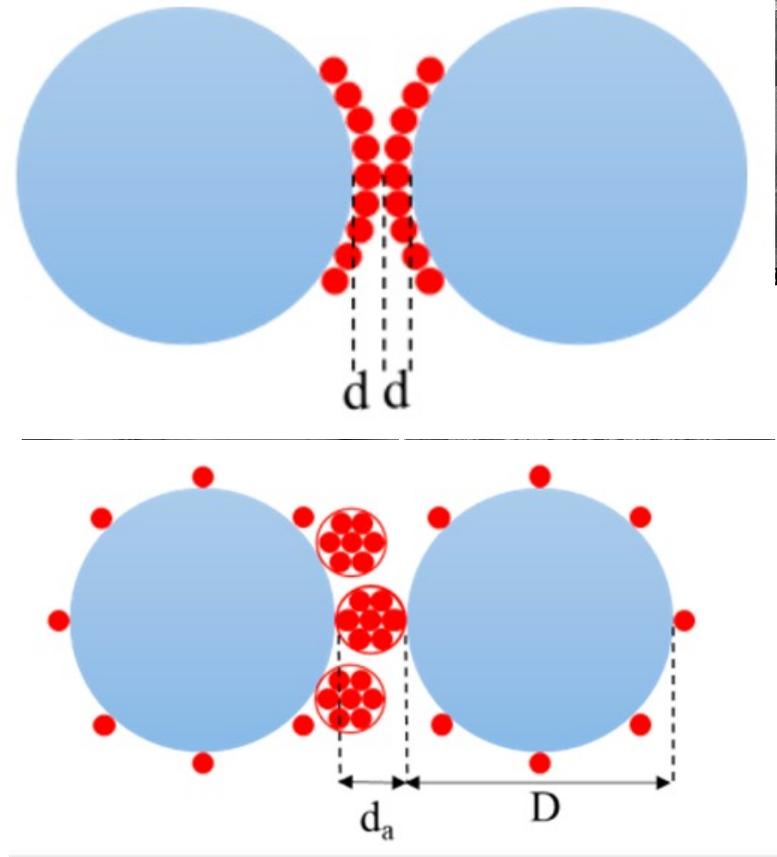
Applying Zheng stick-bounce model
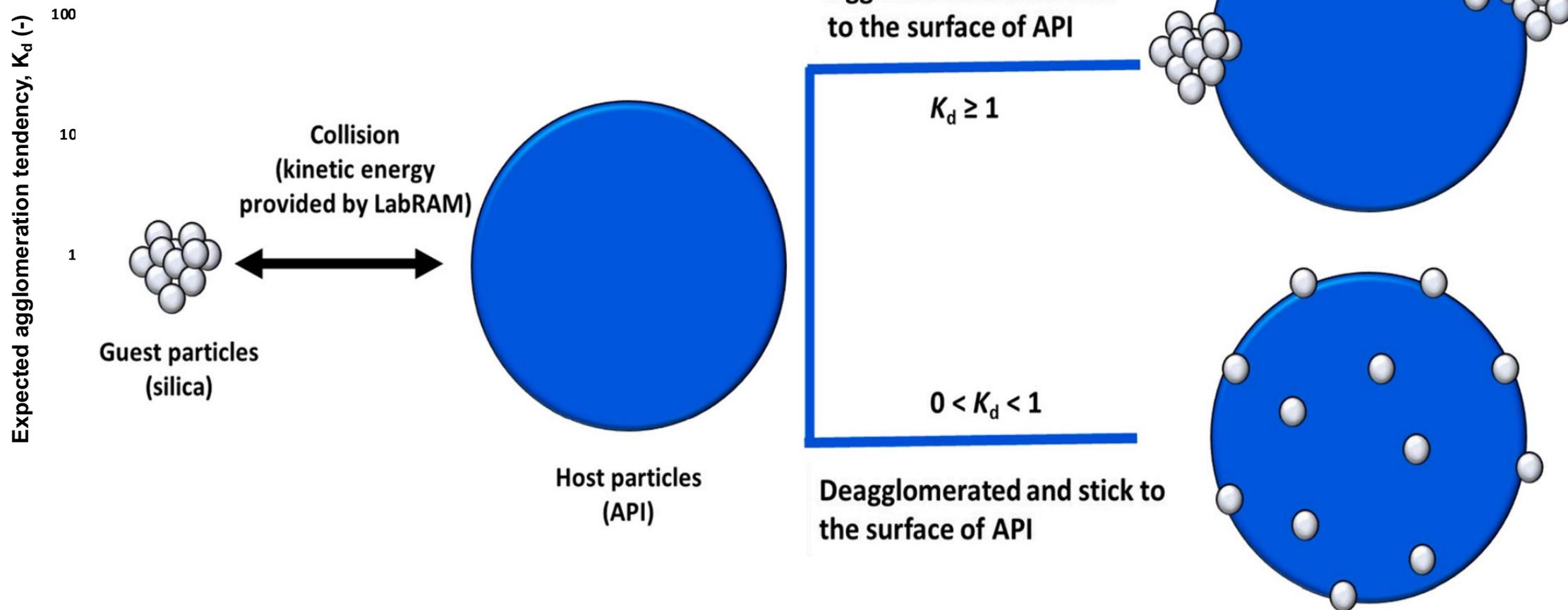
- Agglomeration tendency (K_d)
- Deagglomeration energy (E) / Kinetic energy (E_{kin})

Powder Technology 432

e mass,

Expected agglomeration tendency, K_d (-)

100

10

1

Collision
(kinetic energy
provided by LabRAM)

Guest particles
(silica)

Host particles
(API)

Agglomerated and stick
to the surface of API

$K_d \geq 1$

$0 < K_d < 1$

Deagglomerated and stick to
the surface of API
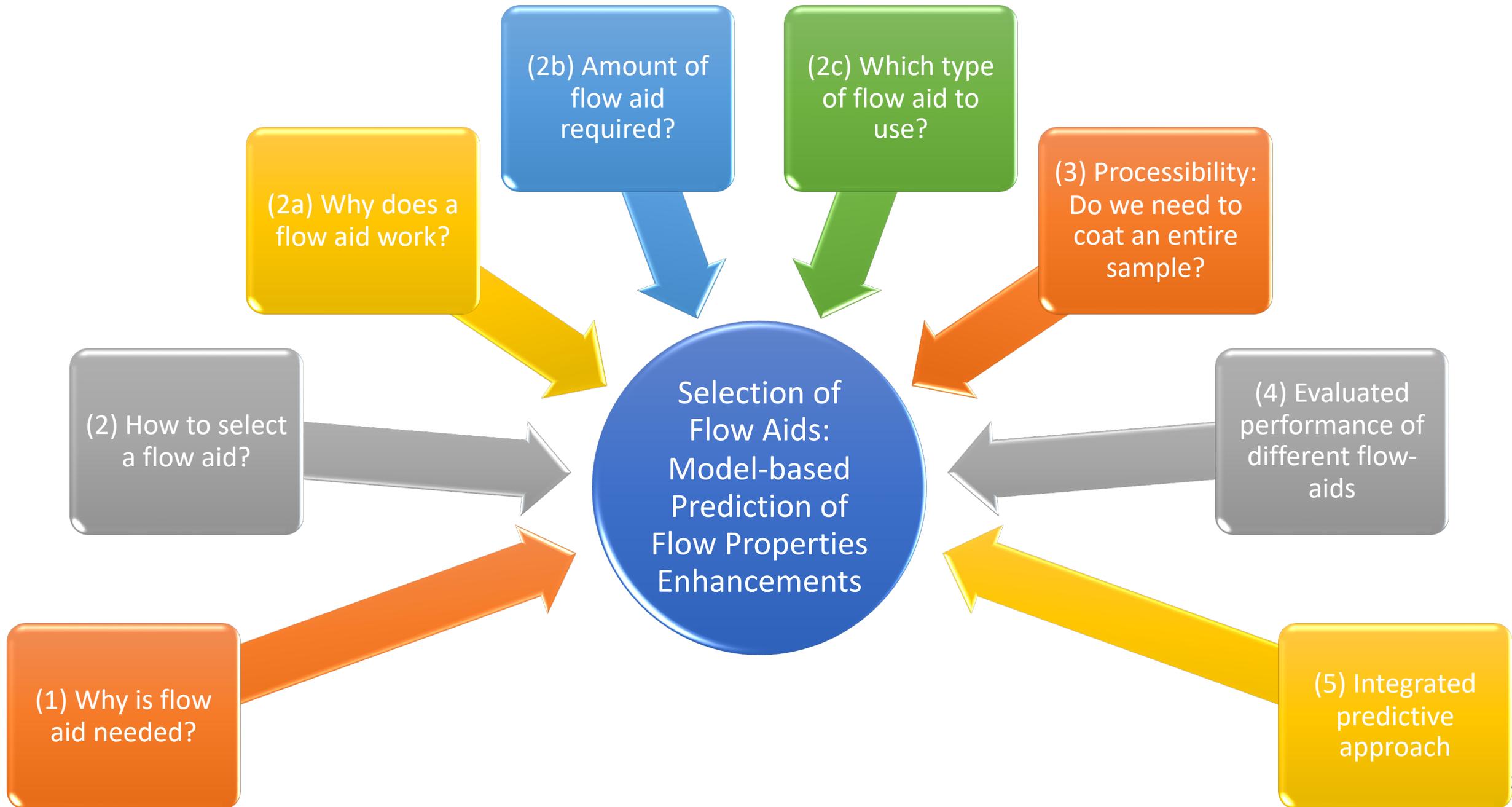
$K_d = f$ (Guest-host contact radius, guest & host van der Waals force, material stiffness, kinetic energy)

Overall Project Achievement: Flow aid guidance

(2b) Amount of flow aid required?

(2c) Which type of flow aid to use?

(2a) Why does a flow aid work?

(3) Processibility: Do we need to coat an entire sample?

(2) How to select a flow aid?

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

(4) Evaluated performance of different flow-aids

(1) Why is flow aid needed?

(5) Integrated predictive approach

20

Key Learnings

Contact model works well even for non-spherical particles that are well-coated powders, however, need to account for:

- PSD effect using the size class dependent Bond number – demonstrated
- Host roughness – ongoing/future
- Silica aggregation – future
- Particle shape - future

Entire batch of powder need not be dry coated

- Possibly as little as 10 wt %.
- Alternately: Finest sized minority component should be dry coated

Flow-aid performance is well explained by integrating assessments based on multiple models

- This needs to be "automated" as a simulation for IFPRI members – ongoing/future

Key Gaps To Address: Renewal Proposal

Improvements in Mechanistic Models

- Limitations of host particle assumptions (spherical, mono-sized, roughness)
- Limitations of guest particle coating assumptions (uniform, monolayer coating)—resulting from device performance
- Integrated simulation package for flow aid guidance and selection

Industry-relevant topics (Experimental)

- Processing device parameters, device performance equivalence map
- Humidity effects on coating process
- Coating stability in downstream processing