

# IFPRI Project #130

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



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IFPRI AGM June 2025

# Progress this year

## Industry-relevant topics

- Processing device parameters and device comparisons
- Scalability to pilot scale
- Effect of flow aid coating on downstream processability

## Model development

- Expansion of the model to account for the host particle size distribution (was included in the annual report)
- Guest particle aggregation vs monolayer uniform dispersion after dry coating based on guest-host interactions due to process dynamics
- Revision of contact model for adhesion considering flow aids aggregation after dry coating
- Accounting for flow aid aggregation morphology on cohesion reduction dynamics
  - Drivers identified – the size of the aggregates as primary effect and the nature of aggregates as the secondary effect
  - Compact spherical aggregates better than lower fractal dimensions aggregates with higher porosity

# Coating device performance

Low Intensity  
Batch Device



V-blender Parameters:

- > Blending Time
- > Intensifier Bar

Medium Intensity  
Continuous Device



Comil Parameters: Residence time

- > Sieve Size
- > Multi-Pass
- > Sieve Blocking

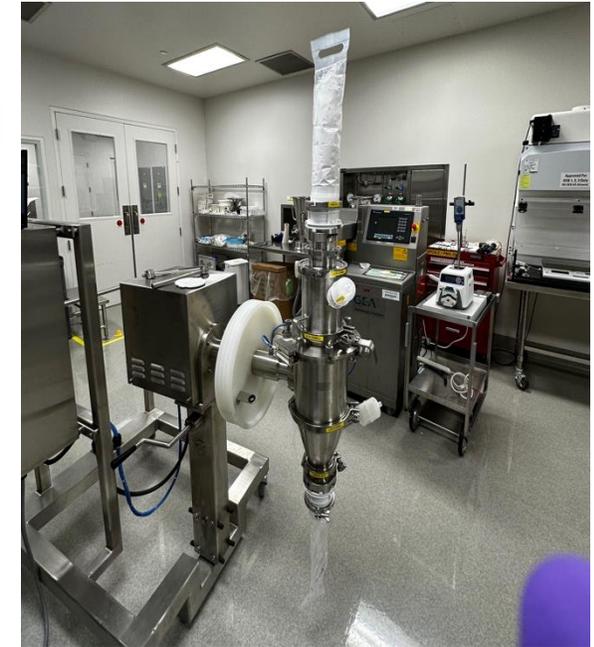
High Intensity  
Batch Device



LabRAM Parameters:

- > Intensity
- > Time

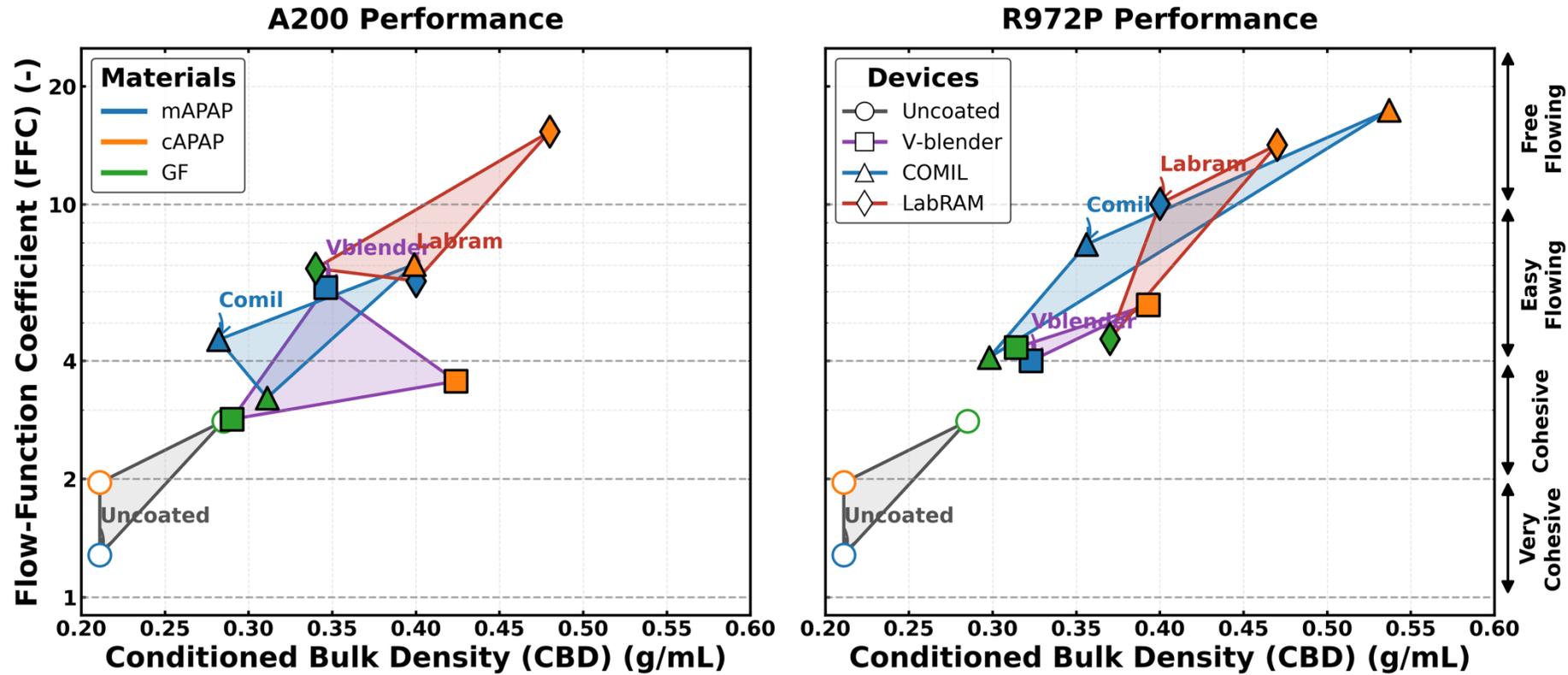
Pilot Scale  
comil (10-20X)



Comil processing  
and effects on  
downstream  
processibility

# Property improvement comparison

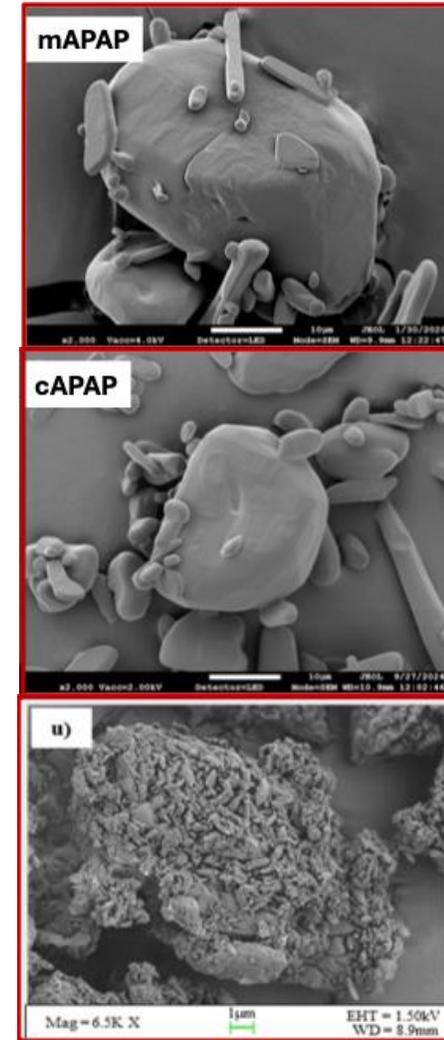
## Comparison of Best Conditions for all Devices



LabRAM generally best

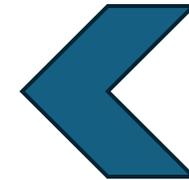
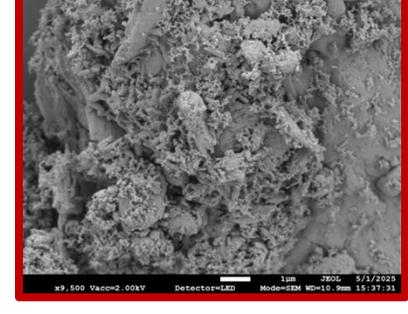
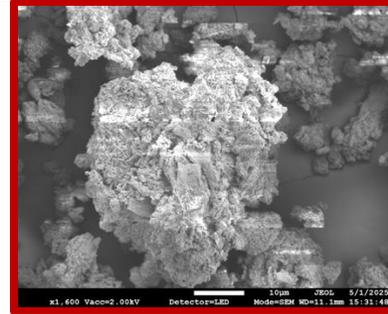
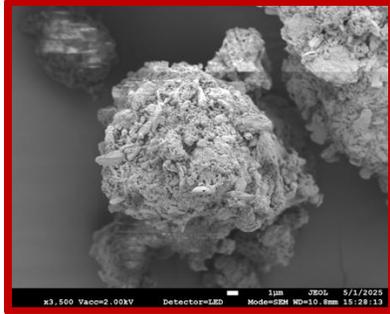
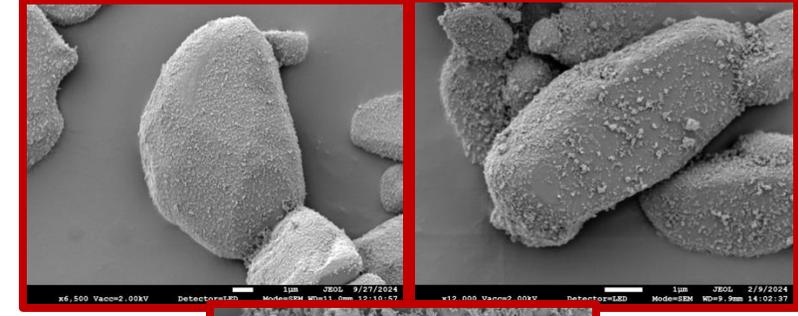
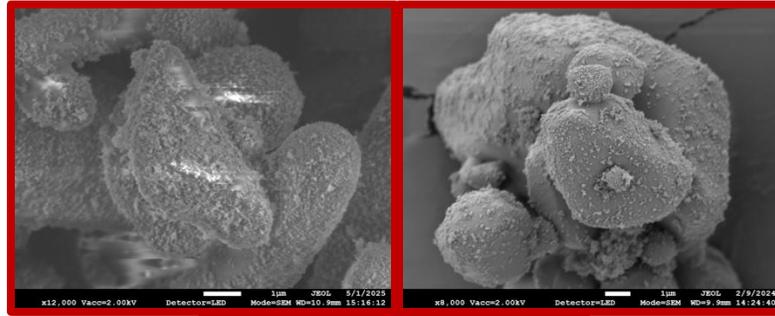
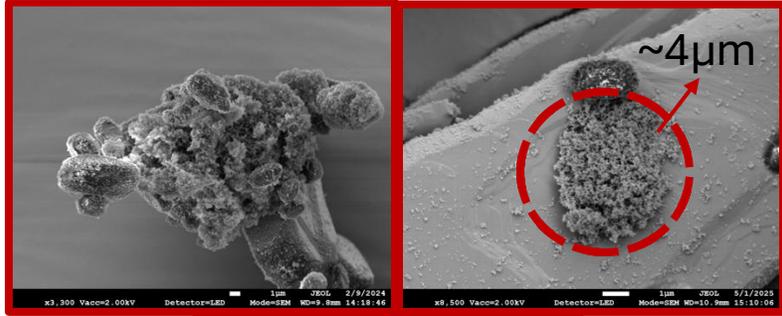
Comil better when optimized

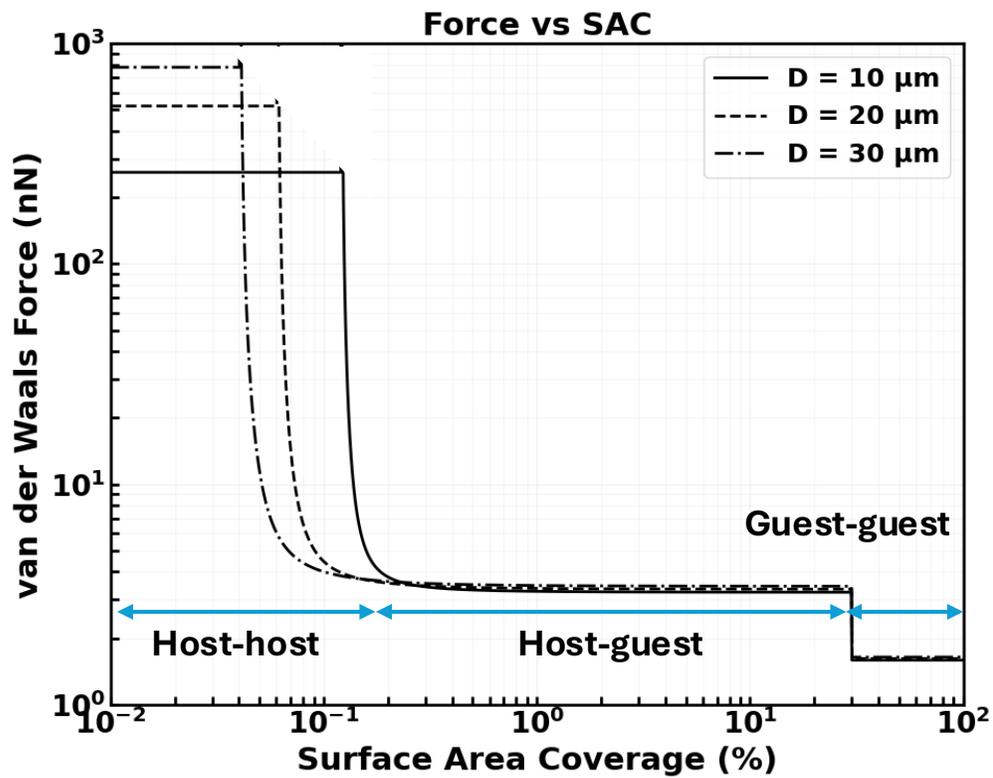
Vblender showed minimum improvements



As received  
Morphology

# Coating quality comparison





vdW force as a function of SAC when the flow aids (guest particles do not appreciably aggregate over the surface of the host particles)

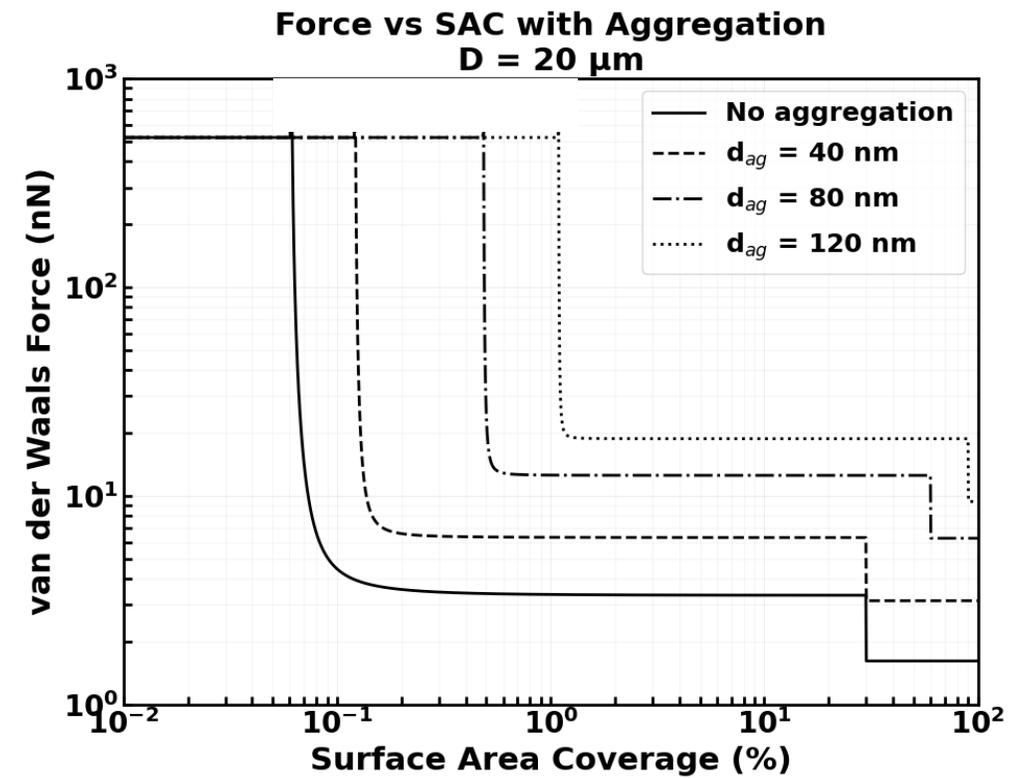
- For a fixed flow aid, the SAC transition from the Host-guest to the guest-guest contacts is not a function of the host particle size
- In contrast, slightly higher SAC is required to reach Host-guest contact regime as the host particle size increases

$$SAC = \frac{N (\pi d^2 / 4)}{4\pi [(d + D) / 2]^2} \times 100\% \approx \frac{Nd^2}{4D^2} \times 100\%.$$

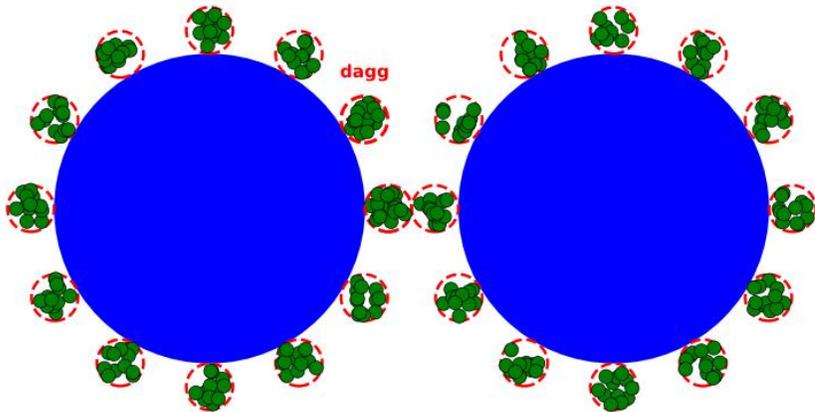
$$F_{ad} = \frac{A * d}{4z_0^2} + \frac{A}{24D \left( \sqrt{\left(1 + \frac{d}{D}\right)^2 - \frac{1.21}{SAC} \left(\frac{d}{D}\right)^2} - 1 \right)^2}$$

vdW force as a function of SAC when the flow aids (guest particles) aggregate significantly over the surface of the host particles

- As may be expected, guest particle aggregation leads to reduction in the effective SAC
- For a fixed flow aid, the SAC transition from the host-guest to guest-guest is a strong function of the guest particle aggregation
- Guest particle aggregation also impacts the SAC transition from host-host to host-guest contact regime as the guest particle aggregate size increases



Assuming spherically packed aggregates

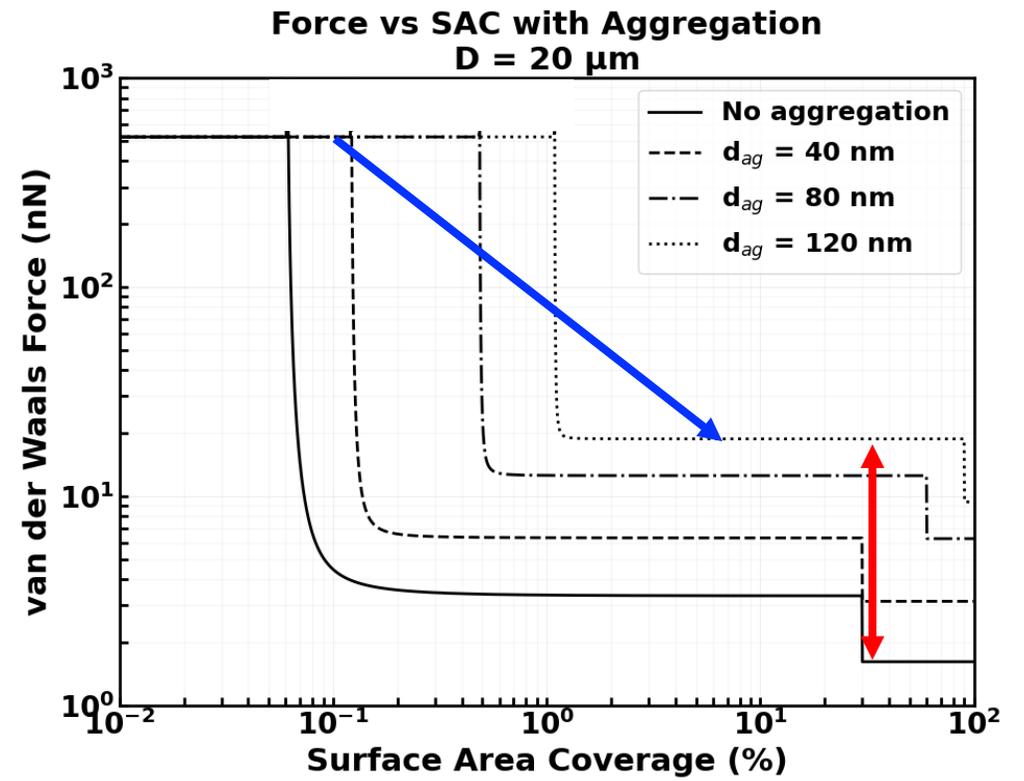
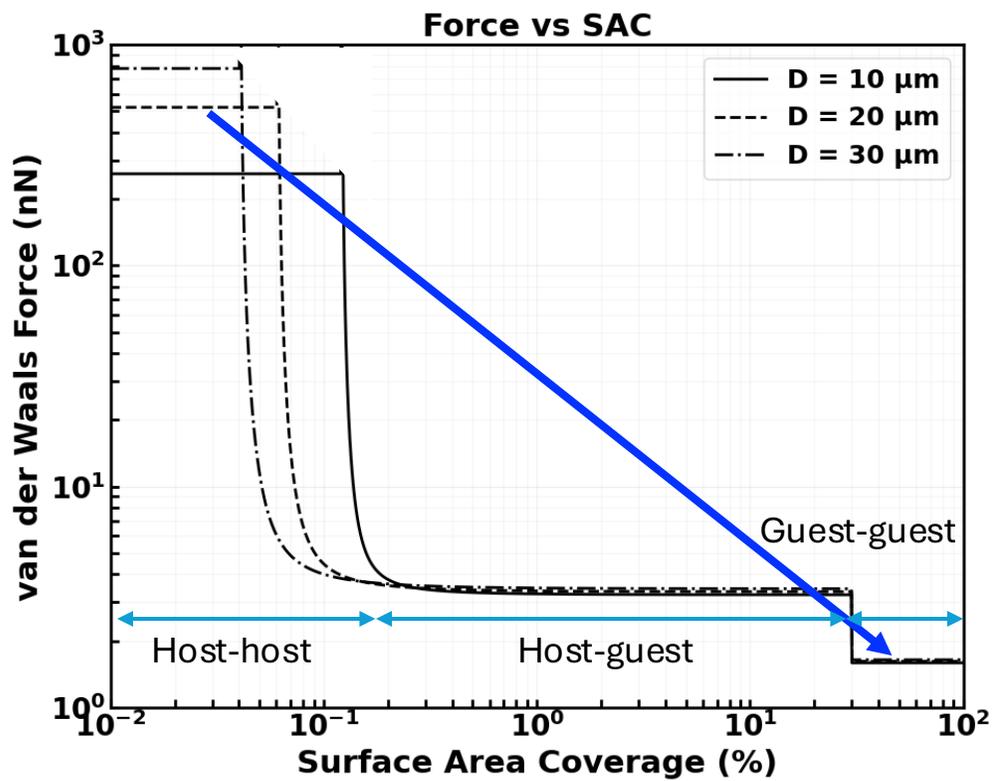


$$F_{ad} = \frac{A * d_{agg}}{4z_0^2} + \frac{A}{24D \left( \sqrt{\left(1 + \frac{d_{agg}}{D}\right)^2 - \frac{1.21}{SAC^*} \left(\frac{d_{agg}}{D}\right)^2} - 1 \right)^2}$$

$$N \frac{\pi}{6} d^3 = N_{ag} \frac{\pi}{6} d_{ag}^3 (1 - \epsilon_{ag}),$$

$$F_{ad} = \frac{A_G}{12z_0^2} \left( \frac{D}{2(H_0/z_0)^2} + \frac{3d_{agg}D}{d_{agg} + D} \right)$$

$$SAC^* = \frac{N_{ag} d_{ag}^2}{4D^2} \times 100\% = \frac{d}{d_{ag} (1 - \epsilon_{ag})} SAC.$$



- As depicted by two blue arrows above, the extent of cohesion reduction is significantly diminished due to aggregation of guest particles or flow aids, which happens more for lower intensity mixing devices. Loss can be up to one order of magnitude (red arrow)
- We need to relate the size of the aggregate ( $d_{agg}$ ) with the number of particles in an aggregate hence the aggregate porosity needs to be estimated, which is done next assuming the aggregates are fractal.

$$F_{ad} = \frac{A * d}{4z_0^2} + \frac{A}{24D \left( \sqrt{\left(1 + \frac{d}{D}\right)^2 - \frac{1.21}{SAC} \left(\frac{d}{D}\right)^2} - 1 \right)^2} \quad \longrightarrow \quad F_{ad} = \frac{A * d_{agg}}{4z_0^2} + \frac{A}{24D \left( \sqrt{\left(1 + \frac{d_{agg}}{D}\right)^2 - \frac{1.21}{SAC^*} \left(\frac{d_{agg}}{D}\right)^2} - 1 \right)^2}$$

$$F_{ad} = \frac{A_G}{12z_0^2} \left( \frac{D}{2(H_0/z_0)^2} + \frac{3dD}{d + D} \right) \quad \longrightarrow \quad F_{ad} = \frac{A_G}{12z_0^2} \left( \frac{D}{2(H_0/z_0)^2} + \frac{3d_{agg}D}{d_{agg} + D} \right)$$

# Flow aid aggregation: Accounting for flow aid aggregate porosity via fractal analysis

Different coating devices or intensities may result in different aggregate structures; here assumed to result into having different fractal dimensions and porosities

$$\varepsilon = 1 - 0.47N_p \left(\frac{k}{N_p}\right)^{\frac{3}{D_f}}$$

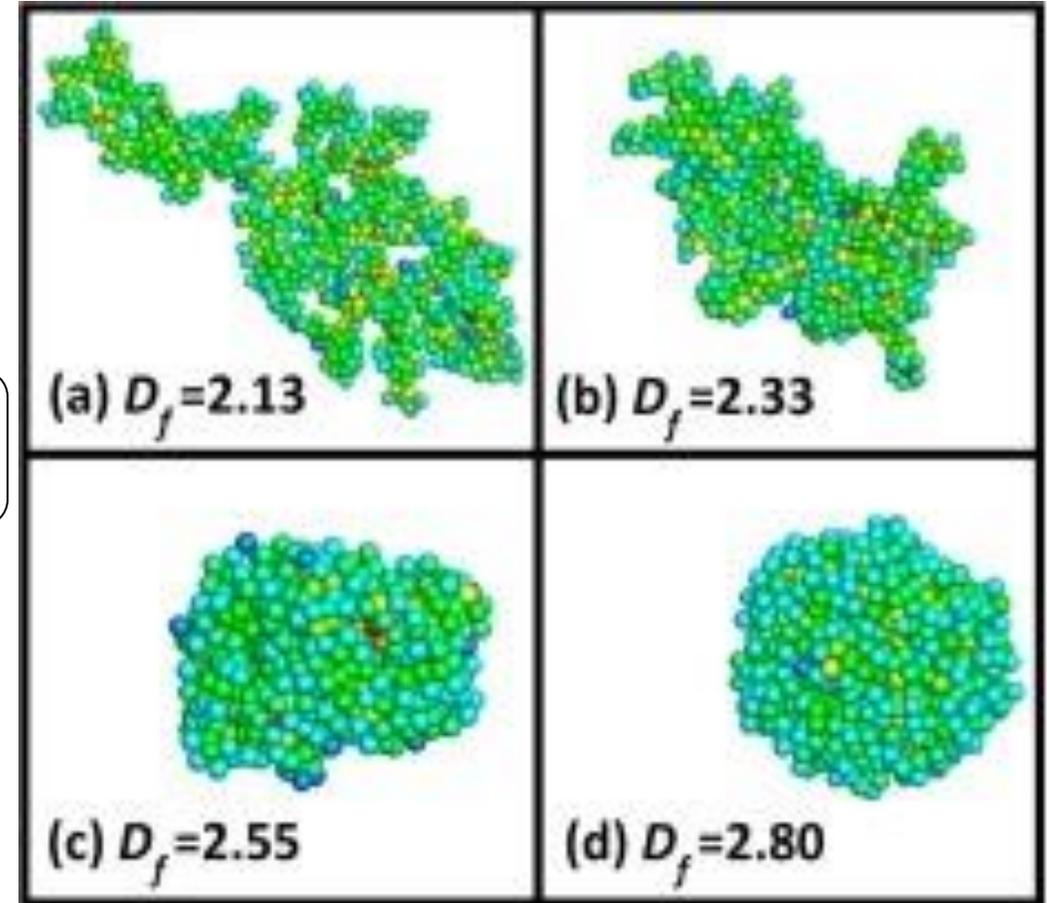
$$N_p = k \left(\frac{R_g}{a}\right)^{D_f}$$

$$D_{agg} = 2 \sqrt{\frac{5}{3}} R_g$$

$$\varepsilon = 1 - 0.47k \left(\frac{\sqrt{3}}{2\sqrt{5}}\right)^{D_f-3} \left(\frac{D_{agg}}{d}\right)^{D_f-3}$$

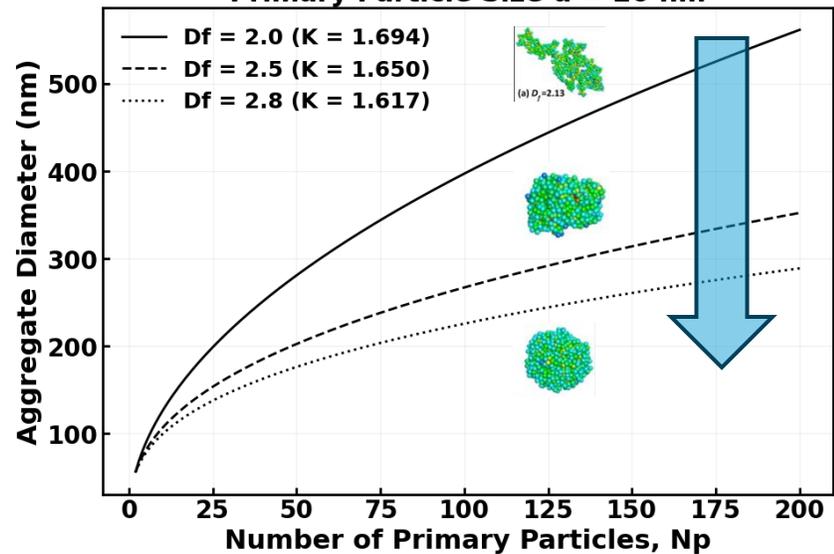


$$\text{Porosity } (\varepsilon) = 1 - \alpha(D_{agg}/d)^\beta$$

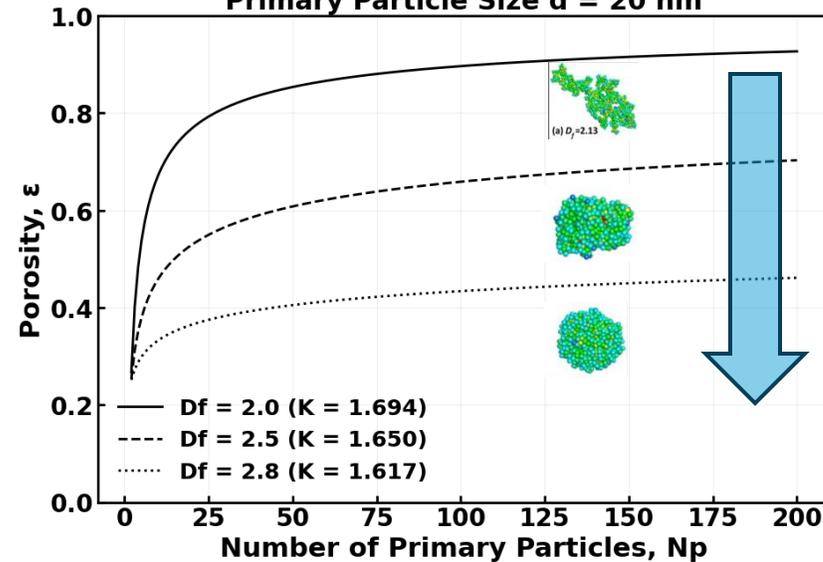


Deng X, Huang Z, Wang W, Davé RN. Investigation of nanoparticle agglomerates properties using Monte Carlo simulations. *Advanced Powder Technology*. 2016;27(5):1971-1979.

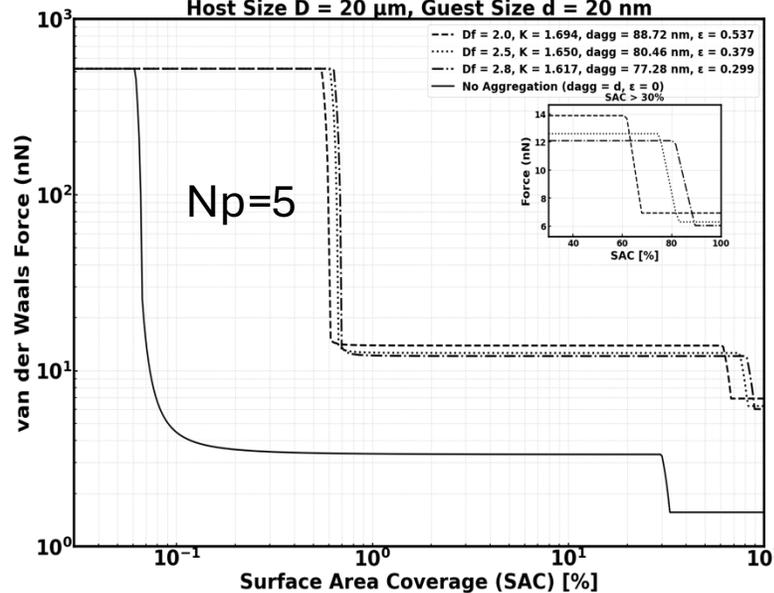
**Aggregate Size vs Number of Particles**  
Primary Particle Size  $d = 20$  nm



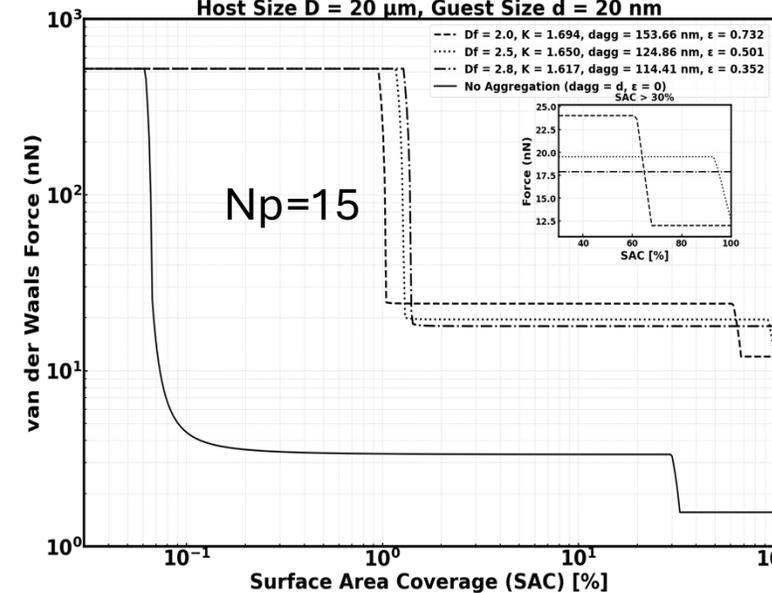
**Porosity vs Number of Particles**  
Primary Particle Size  $d = 20$  nm



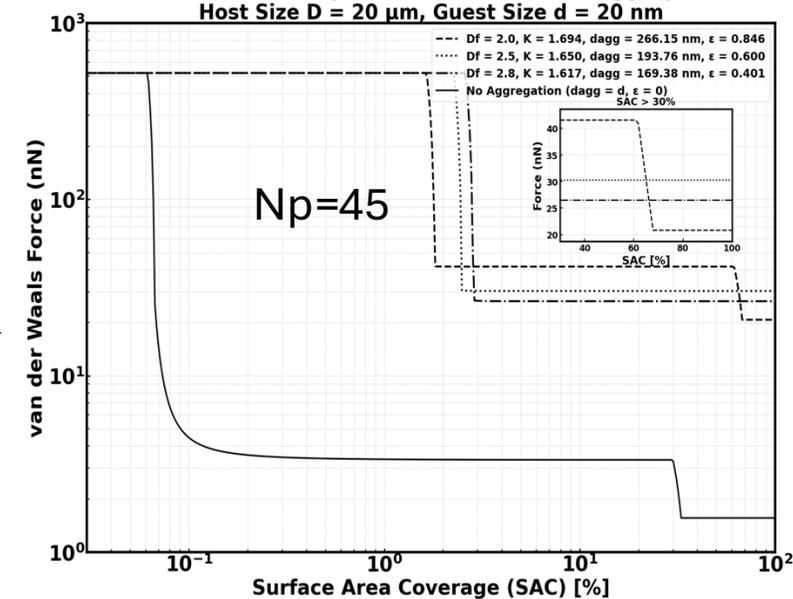
**Force vs SAC for  $N_p = 5$  with and without Aggregation**  
Host Size  $D = 20$   $\mu$ m, Guest Size  $d = 20$  nm



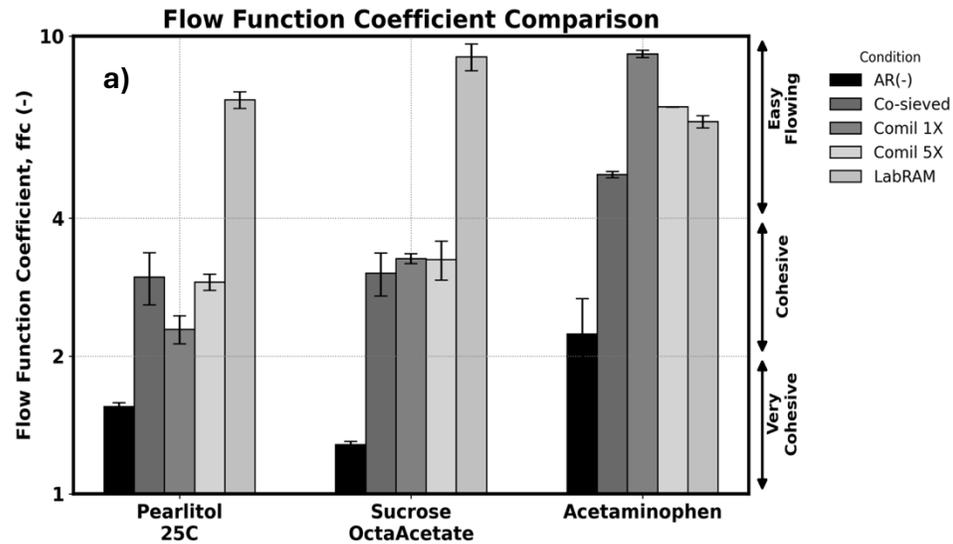
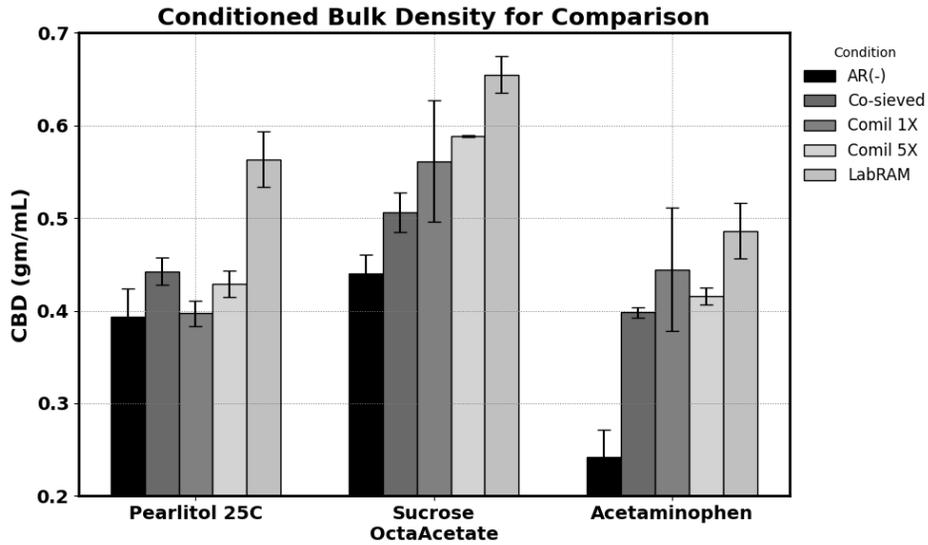
**Force vs SAC for  $N_p = 15$  with and without Aggregation**  
Host Size  $D = 20$   $\mu$ m, Guest Size  $d = 20$  nm



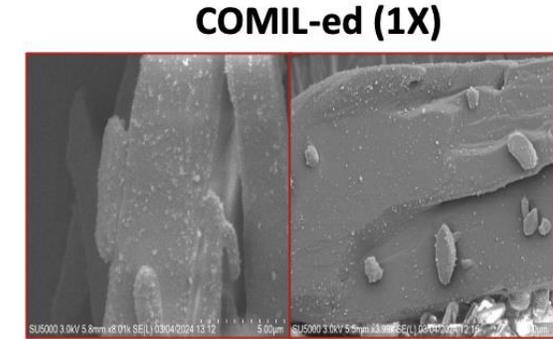
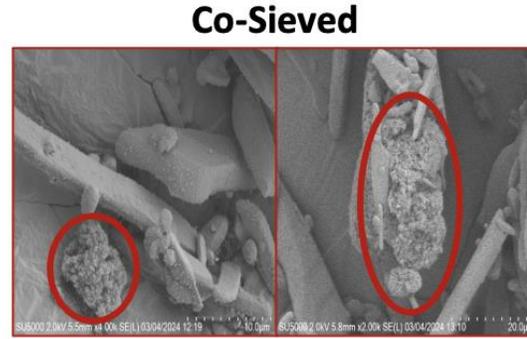
**Force vs SAC for  $N_p = 45$  with and without Aggregation**  
Host Size  $D = 20$   $\mu$ m, Guest Size  $d = 20$  nm



# Pilot Scale Testing: Scalability and Downstream Processability Improvements

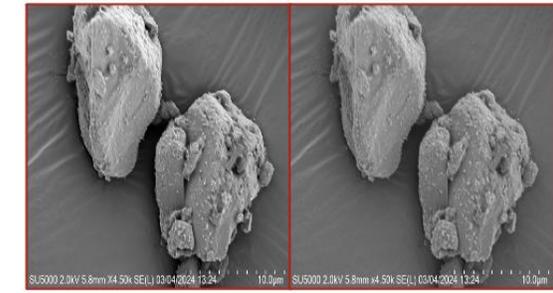
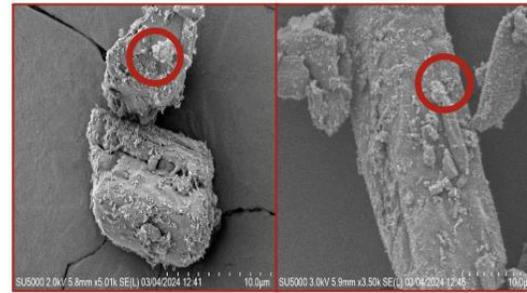


Bulk property comparison for different coating processes



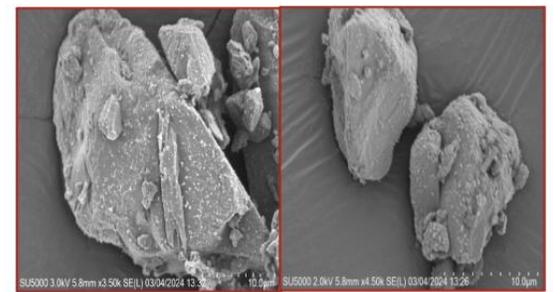
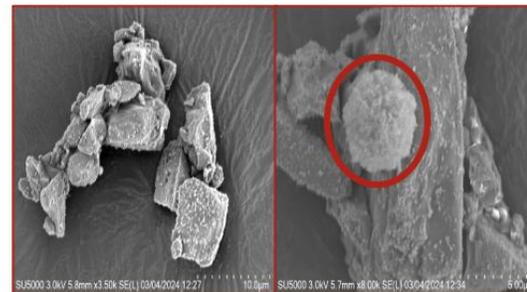
Acetaminophen

Acetaminophen



Pearlitol 25C

Pearlitol 25C



Sucrose Octa Acetate

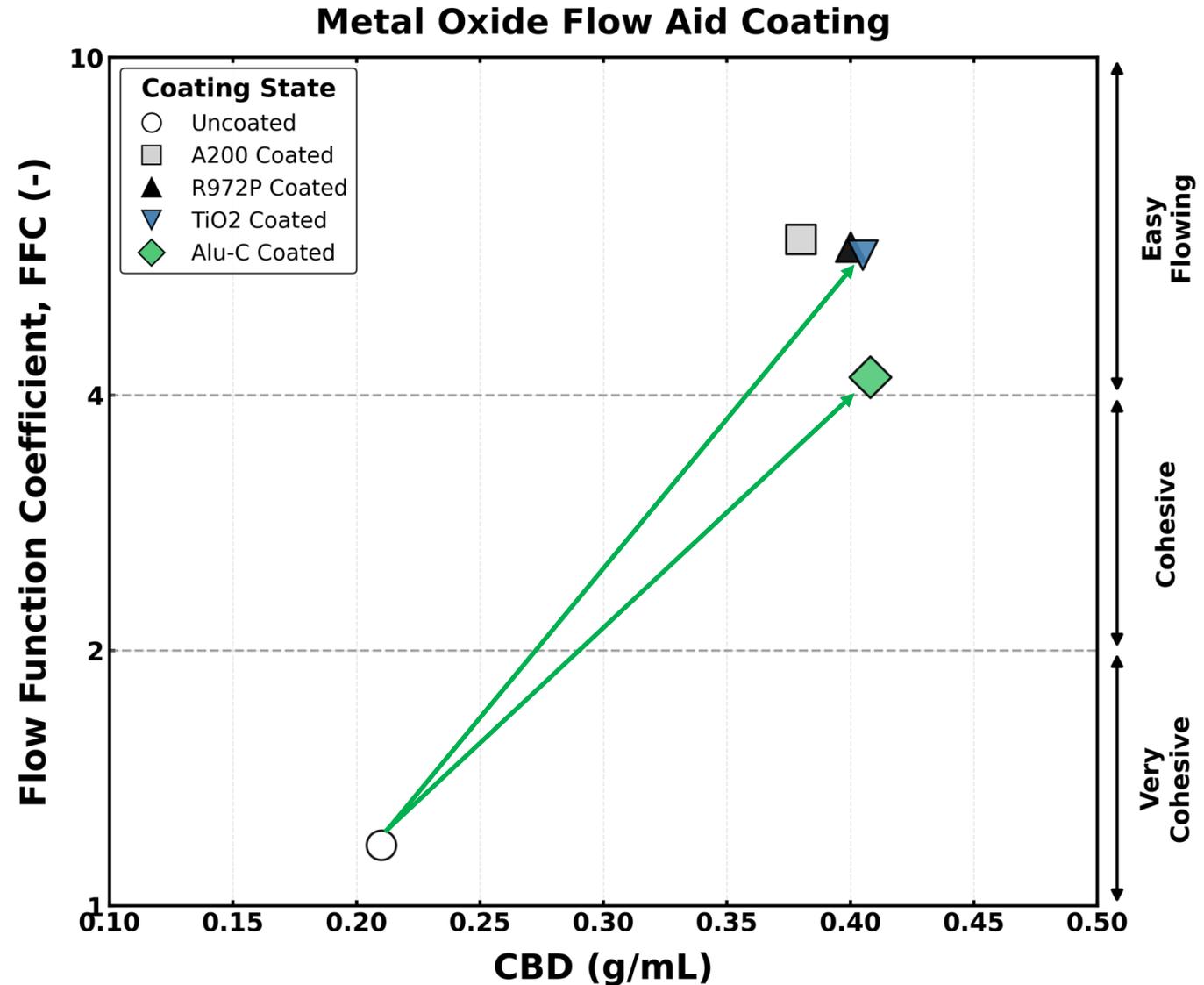
Sucrose Octa Acetate

Better coating quality for comilled

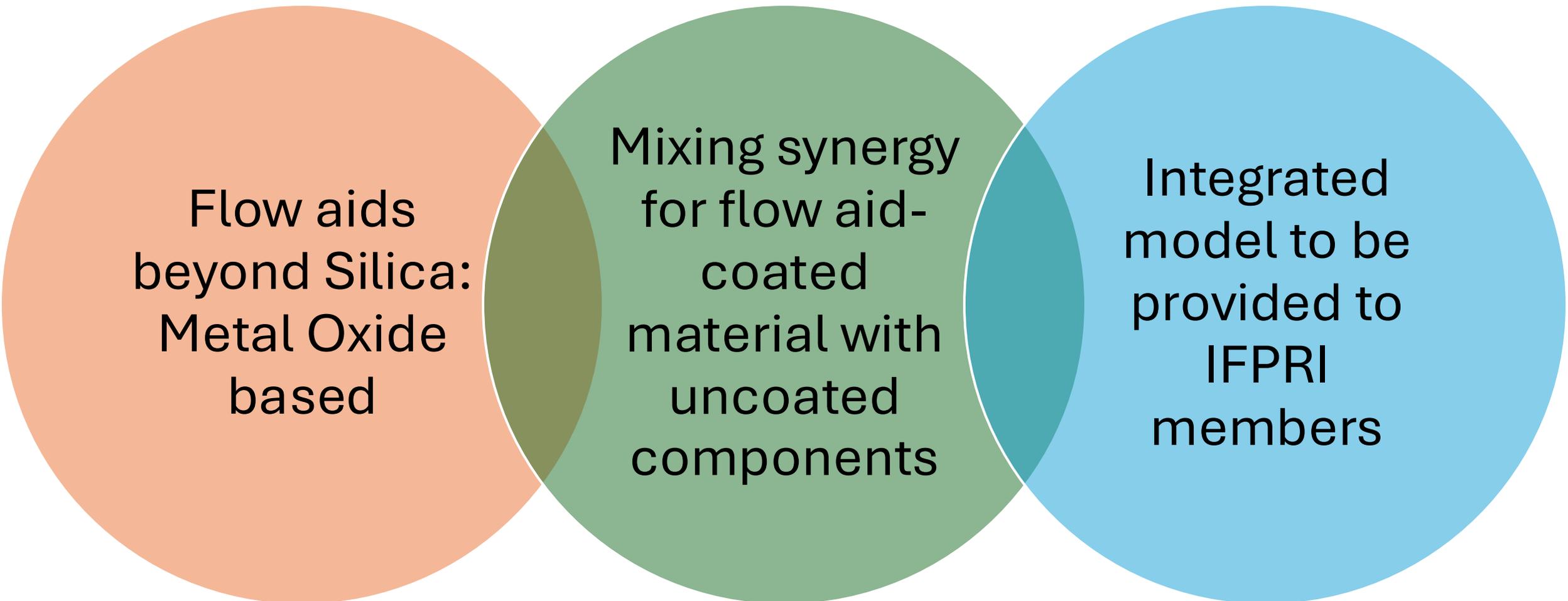
# Dry coating with metal oxide flow aids: $\text{Al}_2\text{O}_3$ & $\text{TiO}_2$

- mAPAP dry coated with 1 wt%  $\text{Al}_2\text{O}_3$  (~30%SAC) &  $\text{TiO}_2$  (16%SAC)
- Works comparable to silica and achieved flow enhancements by two flow regimes:
  - A200 at 50%SAC
  - R972P at 50%SAC

Metal Oxide Properties	Size(d)	Density (kg/m <sup>3</sup> )	$\gamma d$ (J/m <sup>2</sup> )
A200	12nm	2200	42.8
R972P	20nm	2200	36.4
Alu-c	13nm	2710	63.4
TiO <sub>2</sub> (P25)	24nm	4230	14.7



# Current & future activities



Flow aids  
beyond Silica:  
Metal Oxide  
based

Mixing synergy  
for flow aid-  
coated  
material with  
uncoated  
components

Integrated  
model to be  
provided to  
IFPRI  
members