To hinder or to enhance? Clustering and settling behavior of polydisperse, gas-solid flows

E. Foster[★], E.C.P. Breard[♦,◇], S. Beetham[★]

[★] Oakland University, Department of Mechanical Engineering
[♦] University of Edinburgh, School of Geosciences
[◇] University of Oregon, Department of Earth Sciences

Polydisperse gas-solid flows are everywhere

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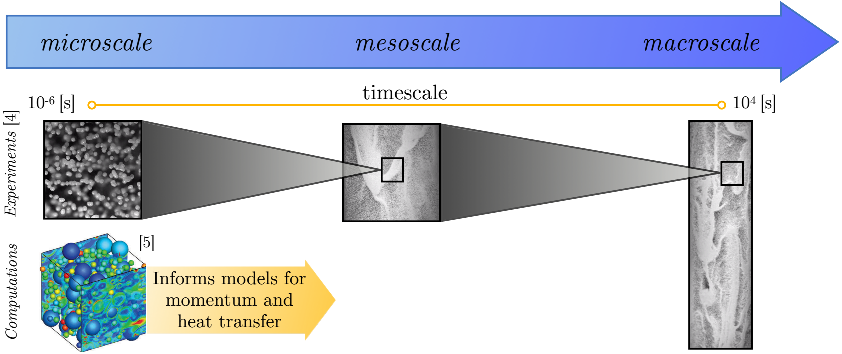
In all real-world applications, the disperse phase is polydispersed!

Computational strategies for gas-solid flows



Particle Resolved DNS

$O(10^3)$ particles

Fully resolves hydrodynamics & heat transfer

Chemical kinetics modeled

Multiphase RANS

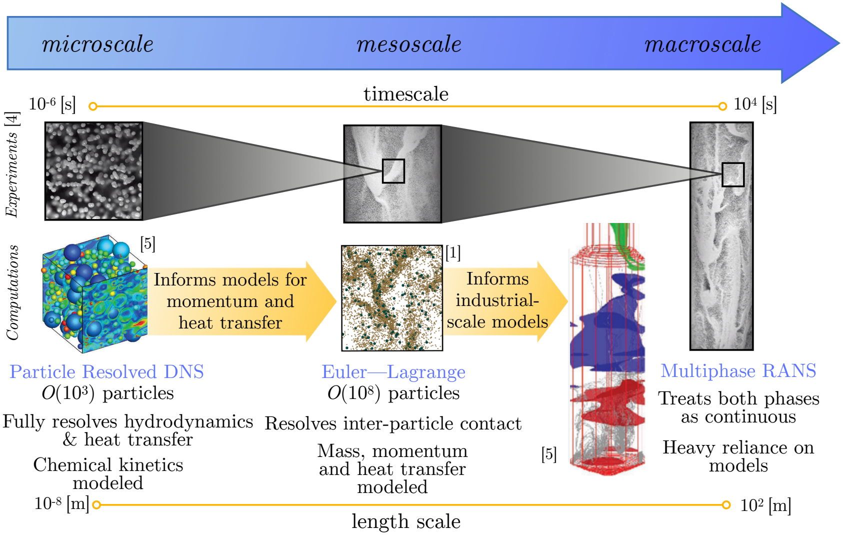
Treats both phases as continuous

Heavy reliance on models

10^{-8} [m] — 10^{2} [m]

length scale

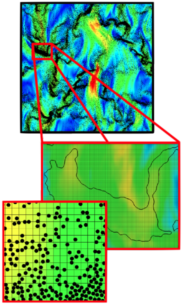
Computational strategies for gas-solid flows



How does polydispersity impact mesoscale clustering & settling behavior?

An Euler–Lagrange approach

Simulations solved using NGA[1]:



- Finite volume DNS/LES code
- Conservation of mass and momentum

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f) = 0$$

$$\frac{\partial}{\partial t}(\alpha_f \rho_f \boldsymbol{u}_f) + \nabla \cdot (\alpha_f \rho_f \boldsymbol{u}_f \boldsymbol{u}_f) = \nabla \cdot \boldsymbol{\tau} + \alpha_f \rho_f \boldsymbol{g} + \mathcal{F}_{\text{inter}}$$

[1] Desjardins et. al (2014)

An Euler–Lagrange approach

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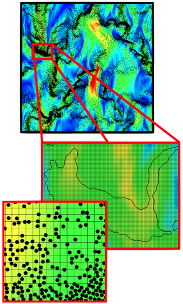

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- Lagrangian particle tracking (Newton's 2nd law)

$$\frac{\mathrm{d}\boldsymbol{x}_p^{(i)}}{\mathrm{d}t} = \boldsymbol{u}_p^{(i)}$$

$$m_p \frac{\mathrm{d}\boldsymbol{u}_p^{(i)}}{\mathrm{d}t} = \boldsymbol{F}_{\text{inter}}^{(i)} + \boldsymbol{F}_{\text{col}}^{(i)} + m_p \boldsymbol{g}$$

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An Euler–Lagrange approach

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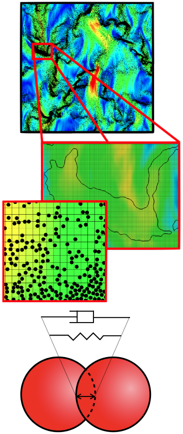

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- Soft sphere collisional model

[1] Desjardins et. al (2014)

An Euler–Lagrange approach

Interphase exchange employs a two-step filtering approach

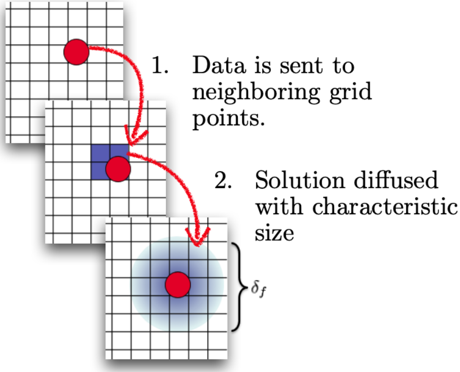
- Volume fraction:

$$\alpha_f = 1 - \sum_{i=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x} - \boldsymbol{x}_p^{(i)}|\right) V_p$$

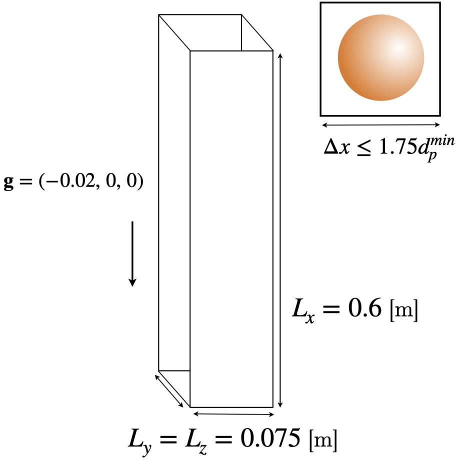
- Momentum exchange

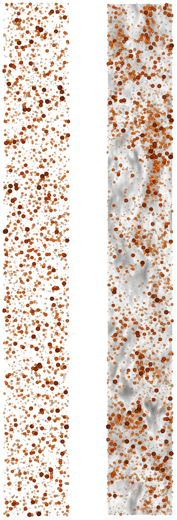
$$\mathcal{F}_{\mathrm{inter}} = -\sum_{i=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x} - \boldsymbol{x}_p^{(i)}|\right) \boldsymbol{f}_{inter}$$

$$\boldsymbol{f}_{\mathrm{inter}} = \underbrace{V_p \nabla \cdot \boldsymbol{\tau}_f}_{\text{resolved}} + \underbrace{m_p \frac{\alpha_f}{\tau_p}\left(\boldsymbol{u}_f - \boldsymbol{u}_p^{(i)}\right) F(\alpha_f, \mathrm{Re}_p)}_{\text{Tenneti et al. (2013)}}$$



Configurations under study





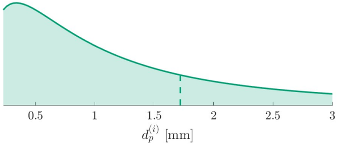
1. *Initial conditions*: $\mathbf{u}_f = 0$ and $\mathbf{u}_p = 0$, particles randomly distributed
2. *Boundary conditions*: Triply periodic

physical parameters

ρ_p	2500	[kg/m^3]
ρ_f	0.50	[kg/m^3]
μ_f	1.85×10^{-5}	[kg/(m s)]
$\boldsymbol{g}$	(-0.02, 0, 0)	[m/s^2]

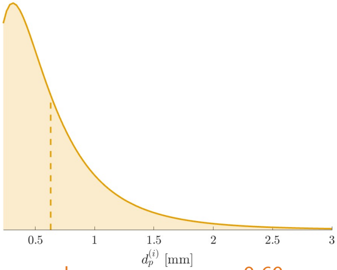
Configurations under study

Distribution A



log normal parameters	μ	0.00
	σ	1.04
cutoff diameters	$d_{p,min}$	0.23 mm
	$d_{p,max}$	3.00 mm
volume fraction	$\langle \alpha_p \rangle$	(0.01, 0.10)
Number of particles	N_p	(19 627, 198 369)

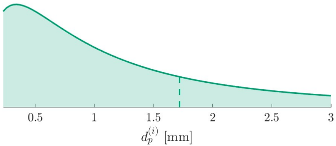
Distribution B



log normal parameters	μ	-0.69
	σ	0.69
cutoff diameters	$d_{p,min}$	0.23 mm
	$d_{p,max}$	3.00 mm
volume fraction	$\langle \alpha_p \rangle$	(0.01, 0.10)
Number of particles	N_p	(75 695, 747 431)

Configurations under study

Distribution A



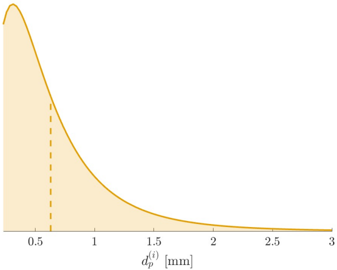
We also consider *mono*disperse 'sister' configurations, A_0, with

$d_p = \exp\left(\mu + \frac{\sigma^2}{2}\right) = 1.72$ at

$\langle \alpha_p \rangle = (0.01, 0.10)$

$N_p = (12\,790, 127\,898)$

Distribution B



We also consider *mono*disperse 'sister' configurations, B_0, with

$d_p = \exp\left(\mu + \frac{\sigma^2}{2}\right) = 0.64$ at

$\langle \alpha_p \rangle = (0.01, 0.10)$

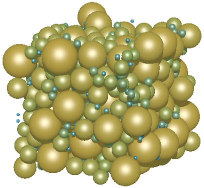
$N_p = (251\,876, 2\,518\,757)$

Configurations under study

Random close packing efficiency[2] is a useful point of reference. This quantity tends to **increase** with **polydispersity**.

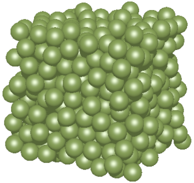
Distribution A

Dist. A



$\alpha_{RCP}^{A} = 0.68$

Dist A_0

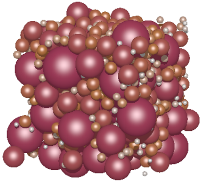


$\alpha_{RCP}^{A_0} = 0.64$

0.23 mm 3.00 mm

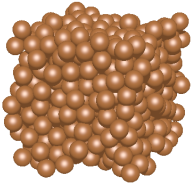
Distribution B

Dist. B



$\alpha_{RCP}^{B} = 0.70$

Dist B_0

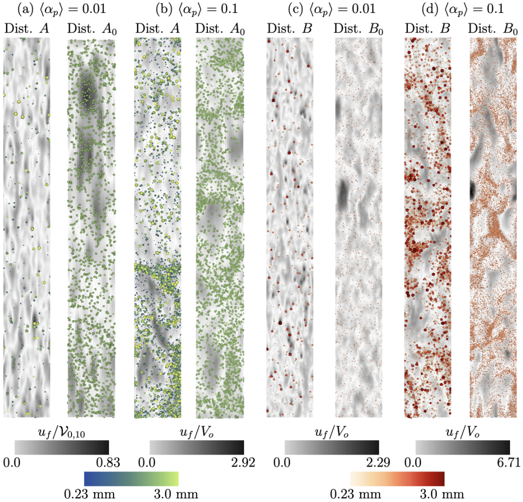


$\alpha_{RCP}^{B_0} = 0.64$

0.23 mm 3.00 mm

[2] Farr (2013), visualizations by KTS algorithm, Kansal et. al (2002)

Heterogeneity emerges after an initial transient



- Due to two-way coupling and heterogeneity spontaneously arises
- After an initial transient, all flows become statistically stationary
- All analysis uses the stationary data

Polydisperse clustering behavior

First, we consider **global** clustering parameters, such as the variance of volume fraction, $\sqrt{\langle \alpha_p'^2 \rangle} / \langle \alpha_p \rangle$.

$\langle \alpha_p \rangle$	Dist	$\sqrt{\langle \alpha_p'^2 \rangle} / \langle \alpha_p \rangle$	φ
0.01	A_0	0.42	50.3
	A	0.87	
	B_0	0.49	
	B	1.34	

$\langle \alpha_p \rangle$	Dist	$\sqrt{\langle \alpha_p'^2 \rangle} / \langle \alpha_p \rangle$	φ
0.10	A_0	0.68	552.7
	A	0.69	
	B_0	0.80	
	B	0.78	

☞ Typically, mass loading ($\varphi = (\langle \alpha_p \rangle \rho_p)/(\langle \alpha_f \rangle \rho_f)$) is used as a predictor of clustering.

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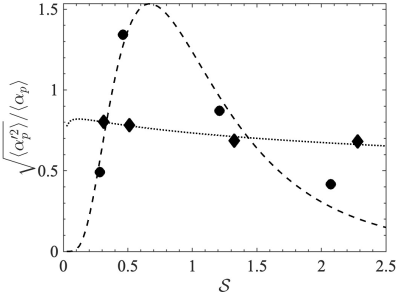
- We find that the degree of clustering varies widely for equivalent mass loading, especially for polydisperse assemblies.
- **A more nuanced metric than mass loading is needed!**

Polydisperse clustering behavior

We propose a new metric to predict degree of clustering, termed 'surface loading', and defined as:

$$\mathcal{S} = \left(\frac{1}{\langle \alpha_f \rangle A_{\text{cross}}}\right)\left(\frac{\rho_p}{\rho_f}\right)\frac{\pi}{4}\frac{1}{N_p}\sum_{i=1}^{N_p}\left(d_p^{(i)}\right)^2$$



$\langle \alpha_p \rangle = 0.01$: ○ $\langle \alpha_p \rangle = 0.10$: ◇

- Very small $\mathcal{S}$ represents a very dilute suspension of very fine particles.
- Very large $\mathcal{S}$ represents a very dense suspension of larger particles.
- Variance on volume fraction should asymptotically approach 0 for $\mathcal{S} \to 0$ and $\mathcal{S} \to \infty$

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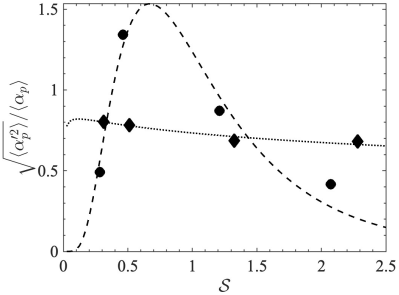


$\langle\alpha_p\rangle = 0.01$: ○ $\langle\alpha_p\rangle = 0.10$: ◇

We propose a model relating $\sqrt{\langle\alpha_p'^2\rangle}/\langle\alpha_p\rangle$ to $\mathcal{S}$:

$$\frac{\sqrt{\langle\alpha_p'^2\rangle}}{\langle\alpha_p\rangle} = \frac{1}{A\,\mathcal{S}}\exp\left(\frac{-(\ln(\mathcal{S})-B)^2}{C}\right)$$

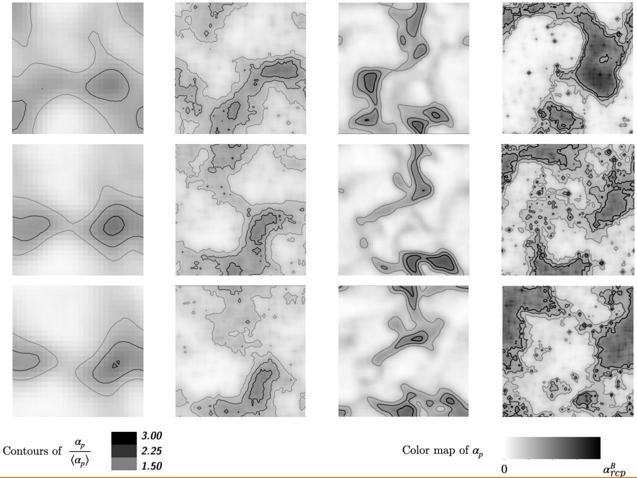
with the coefficients, A, B and C:

$$A = -8.2\langle\alpha_p\rangle + 0.9$$
$$B = 76.0\langle\alpha_p\rangle - 0.8$$
$$C = 164.0\langle\alpha_p\rangle - 0.9.$$

Let's take a more **nuanced** look at clustering behavior.

Polydisperse clustering behavior at $\langle \alpha_p \rangle = 0.10$

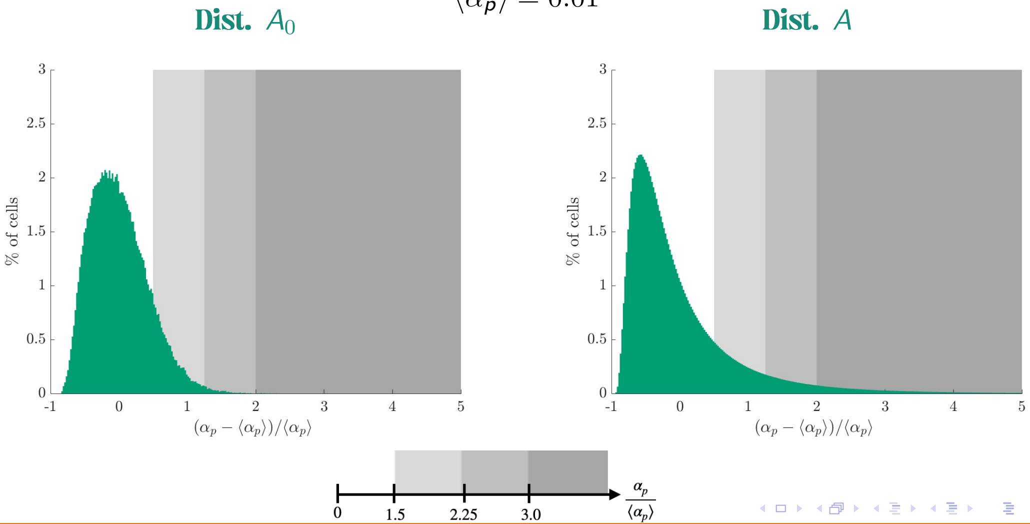
Dist. A_0	Dist. A	Dist. B_0	Dist. B



- Polydisperse configurations exhibit **denser** cluster centers.
- Cluster boundaries are smoother for monodisperse configurations.
- **Dist.** B **and** B_0 achieve exhibit **denser** clustered regions than Dist. A and A_0.

Distributions of particle size by volume fraction

$\langle \alpha_p \rangle = 0.01$



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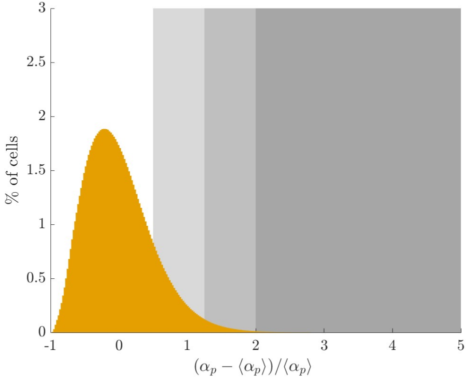
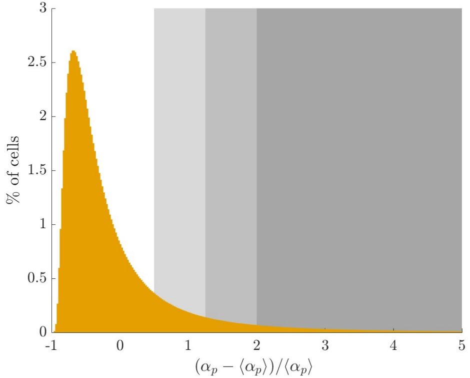
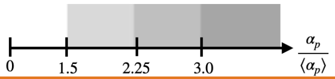
Dist. B_0



Dist. B

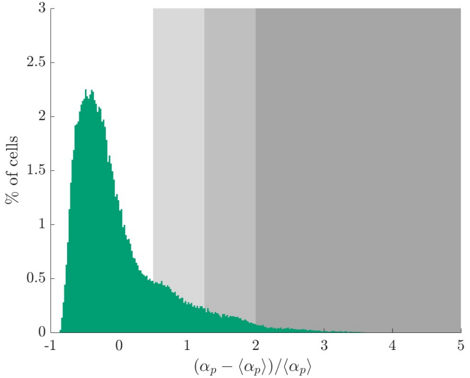




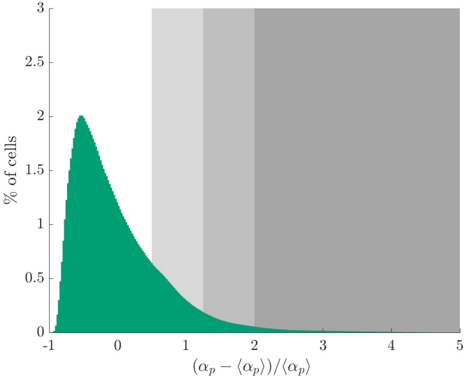
Distributions of particle size by volume fraction

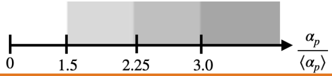
$$\langle \alpha_p \rangle = 0.10$$

Dist. A_0



Dist. A

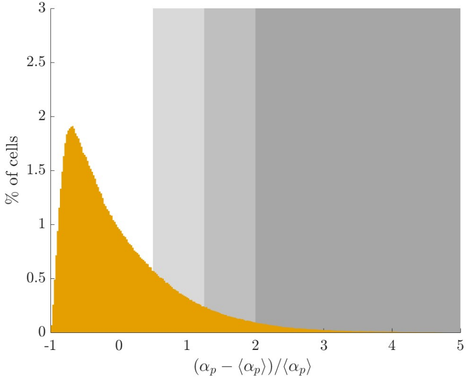




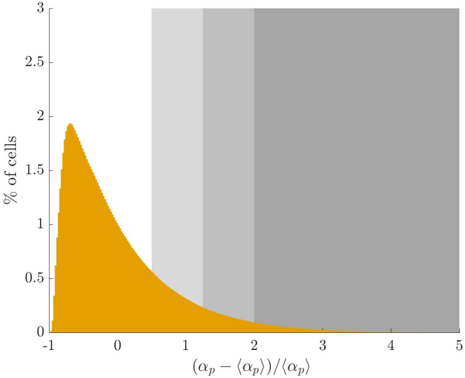
Distributions of particle size by volume fraction

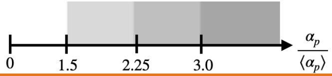
$$\langle \alpha_p \rangle = 0.10$$

Dist. B_0



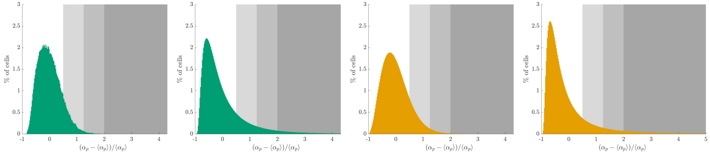
Dist. B



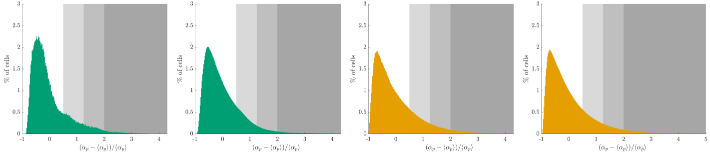


Distributions of particle size by volume fraction

$$\langle \alpha_p \rangle = 0.01$$

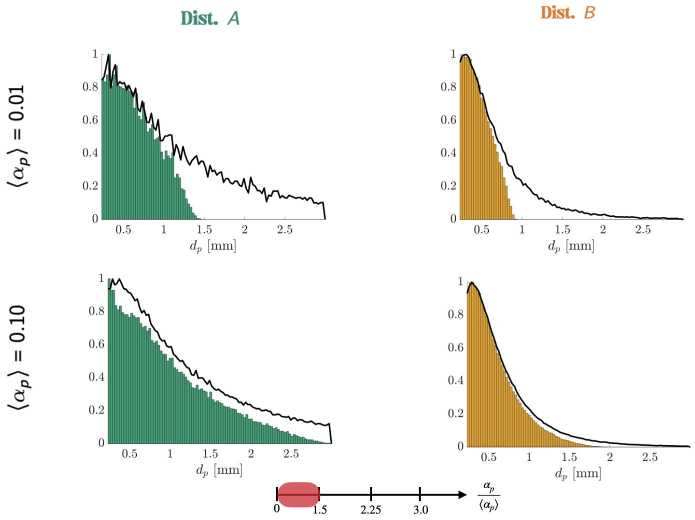


$$\langle \alpha_p \rangle = 0.10$$



- At lower $\langle \alpha_p \rangle$, monodisperse distributions are nearly **Gaussian** and polydisperse are **log normal**.
- At higher $\langle \alpha_p \rangle$, **both** monodisperse and polydisperse are **log normal**

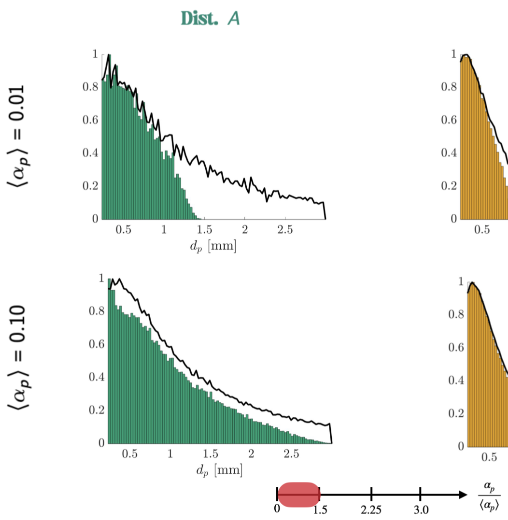
Particle distributions by volume fraction



- Solid lines represent the full domain distribution
- Shaded regions correspond to particles belonging to:

1. dilute, unclustered regions
2. loosely clustered regions
3. moderately clustered regions
4. densely clustered regions

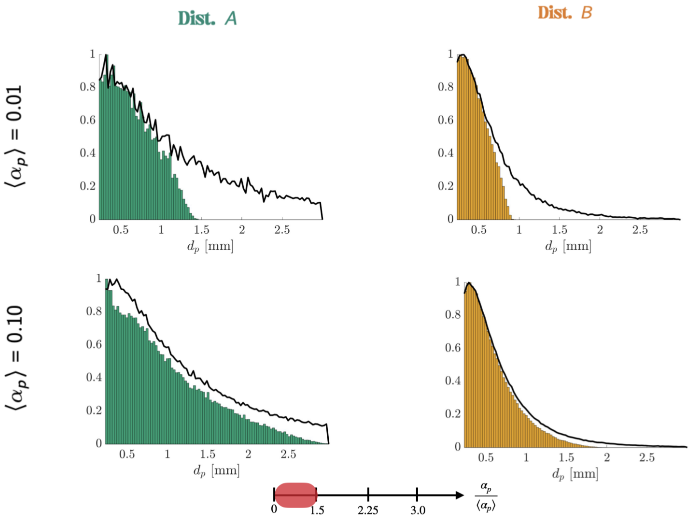
Particle distributions by volume fraction



For the dilute configurations:

- Unclustered regions include **smaller** particles (note: $d_p^{(i)} \leq d_{3,0}$).
- Moderately sized particles dominate the loosely and moderately clustered regions .
- The largest particles can **only be found in the most densely clustered regions**.
- This suggests that it is the largest particles that generate clusters.

Particle distributions by volume fraction



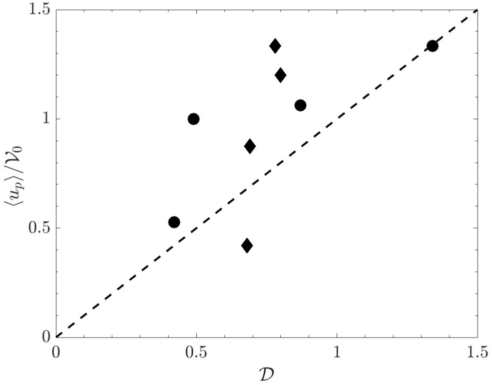
For the denser configurations:

- Unclustered regions *exclude* the largest particles.
- The moderately clustered regions begin to include larger particles
- The densest regions of clusters have greater proportions of large compared with small particles
- Denser suspensions have more blended cluster structures.

How does clustering behavior impact settling behavior?

Traditional methods are not very predictive

Traditionally, the parameter $\mathcal{D} = \sqrt{\langle \alpha_p'^2 \rangle} / \langle \alpha_p \rangle$ has been used to both quantify degree of clustering as well as settling behavior.



- The use of $\mathcal{D}$ is not directly useful for predicting mean settling velocity.
- Recall that we introduced a surface loading $\mathcal{S}$ to predict degree of clustering, rather than mass loading.

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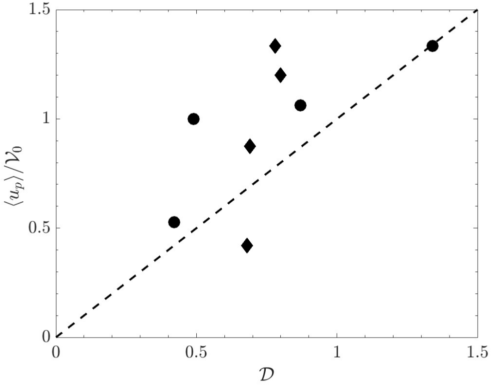

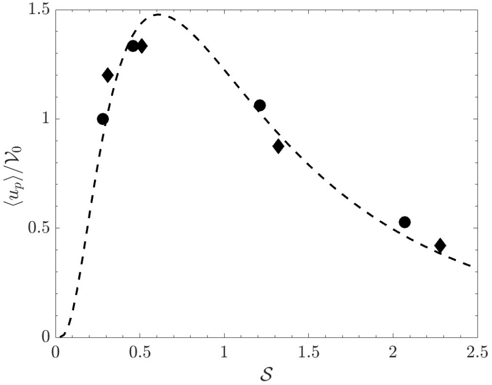

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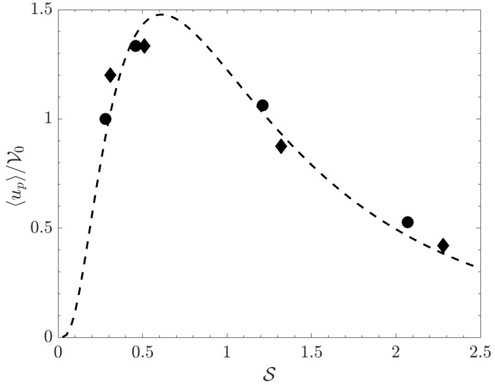
Traditionally, the parameter $\mathcal{D} = \sqrt{\langle \alpha_p'^2 \rangle} / \langle \alpha_p \rangle$ has been used to both quantify degree of clustering as well as settling behavior.

The model connecting $\langle u_p \rangle$ to $\mathcal{S}$ is:

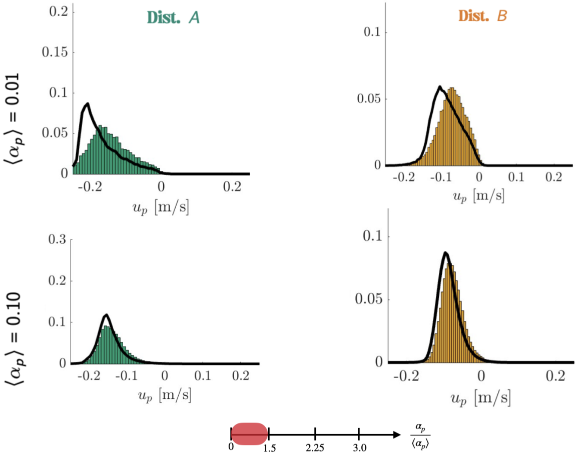
$$\frac{\langle u_p \rangle}{\mathcal{V}_0} = \frac{2.5}{\left(B\mathcal{S}\sqrt{2\pi}\right)} \exp\left(-\frac{(\ln(\mathcal{S}) - A)^2}{2B^2}\right)$$

where $A = 0.15$ and $B = 0.8$



A more nuanced look at settling

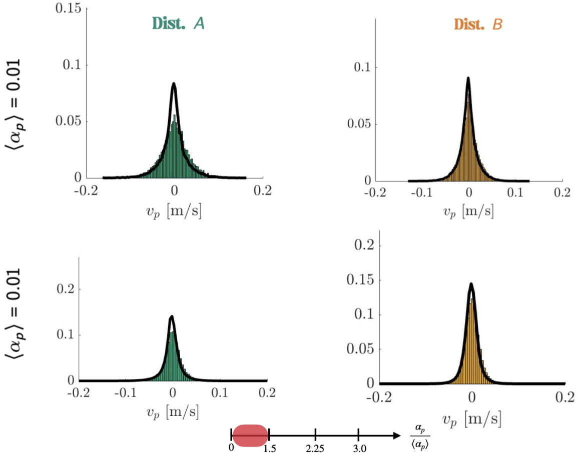
How does settling behavior change depending on local volume fraction?



- Particles in the most dilute region have smaller velocities. This is more pronounced in the dilute cases.
- As local volume fraction increases, particles attain higher velocities.

A more nuanced look at settling

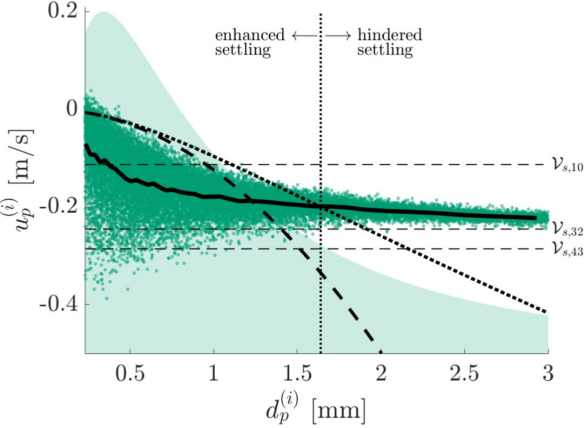
How does cross-stream velocity change depending on local volume fraction?



- Particles in the most dilute region have wider spread velocities, indicating higher granular temperature.
- As local volume fraction increases, particles attain velocities closer to null.

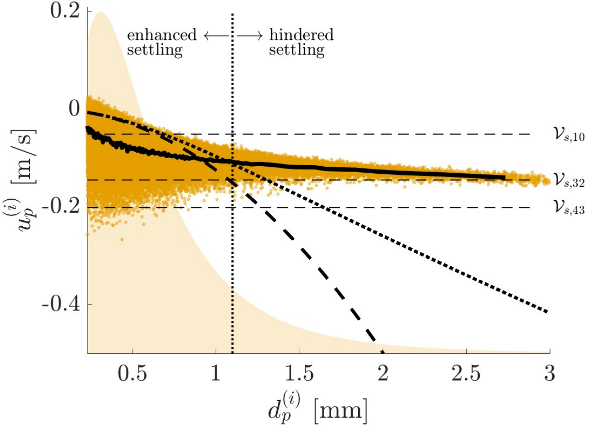
Settling velocity as a function of particle size

Dist. A



$\langle \alpha_p \rangle = 0.01$

Dist. B



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Settling velocity as a function of particle size

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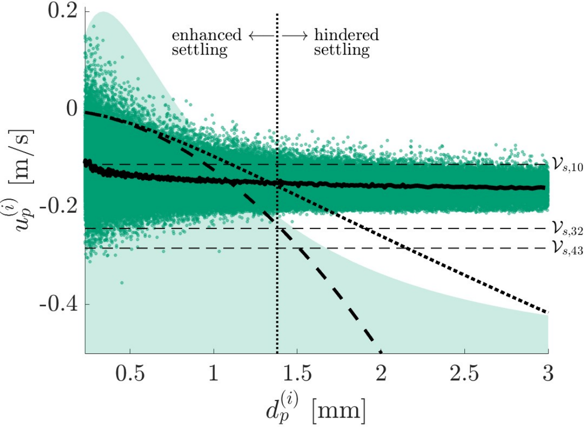
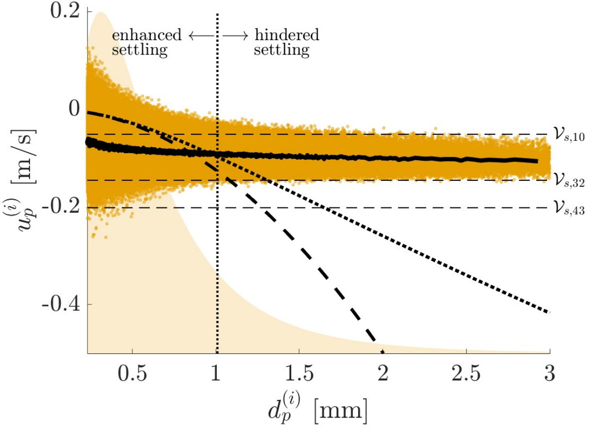


$\langle \alpha_p \rangle = 0.10$

Dist. B



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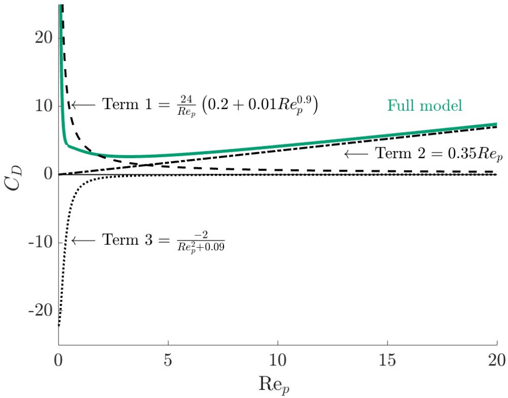
An improved modeling for settling velocity

We propose a **new model** for C_D to improve the prediction for settling velocity.



$$\mathbb{V}_s = \sqrt{\frac{4}{3C_D} g d_p \left(\frac{\rho_p - \rho_f}{\rho_f}\right)}$$

$$\mathbb{C}_D = \frac{24\ C}{D\ \mathrm{Re}_p}\left(0.2 + 0.01\left(D\mathrm{Re}_p\right)^{0.9}\right) + 0.35 CD\ \mathrm{Re}_p - \frac{2}{\left(D\mathrm{Re}_p\right)^2 + 0.09} + \frac{E\ \mathcal{W}}{1 + \mathrm{Re}_p^2}$$

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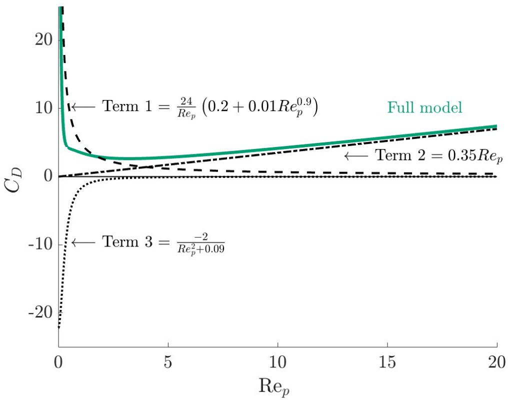

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$\langle\alpha_p\rangle$	Distribution	C	D	E
0.01	A_0	1.25	1.00	–
	A	1.00	1.00	5.00
	B_0	14.00	1.00	–
	B	3.50	1.00	5.00
0.10	A_0	1.25	3.00	–
	A	1.00	2.50	0.10
	B_0	10.00	3.00	–
	B	2.20	5.00	5.00

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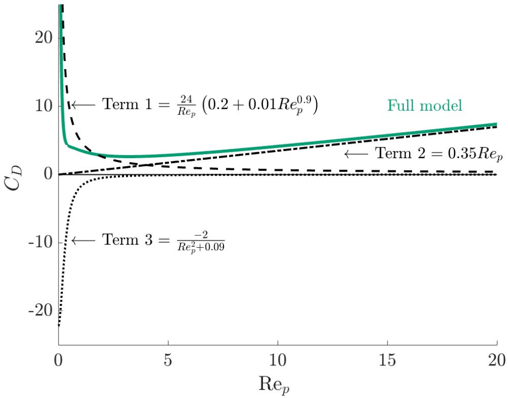

What does each of these terms do?

Term 1 is a modification of the model of Gidaspow (1994).

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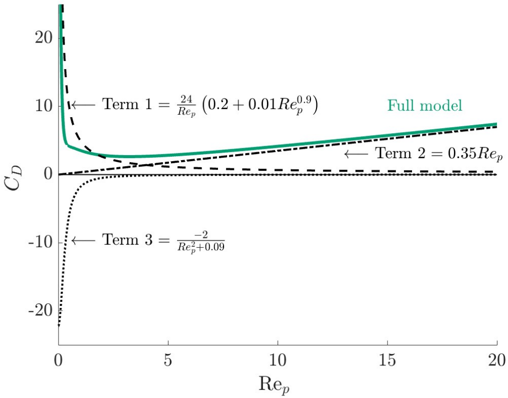

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- **Term 2** accounts for reduced drag felt by larger particles that are embedded in clusters.

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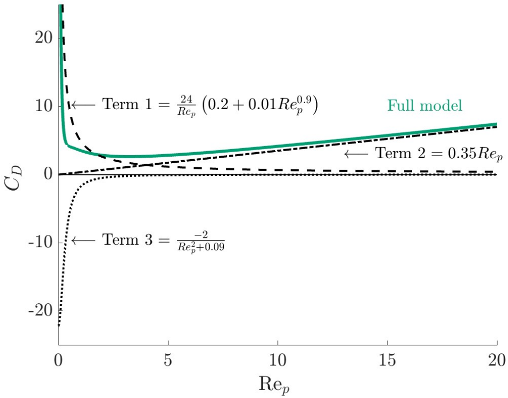

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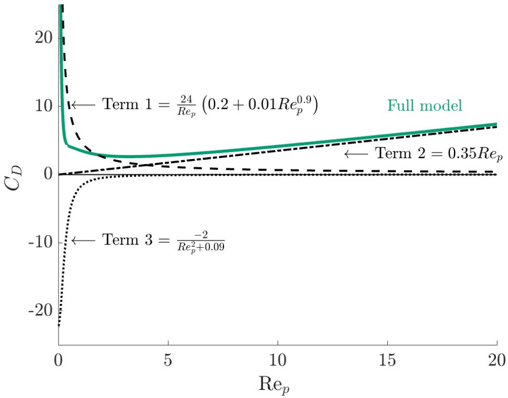

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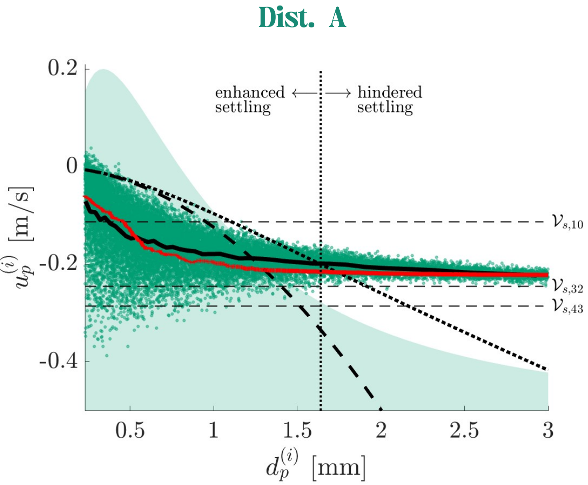
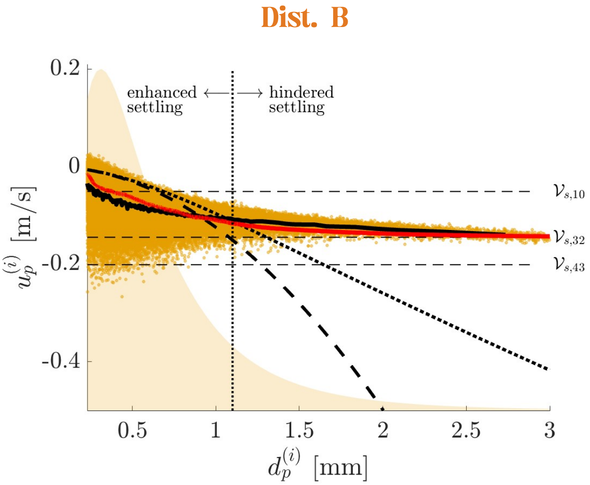
- **Term 2** accounts for reduced drag felt by larger particles that are embedded in clusters.
- **Term 3** adjusts for the increased drag felt by larger particles due to clustering.
- **Term 4** introduces stochasticity in the model through a Weiner process, $\mathcal{W}$.

An improved modeling for settling velocity



$\langle \alpha_p \rangle = 0.01$



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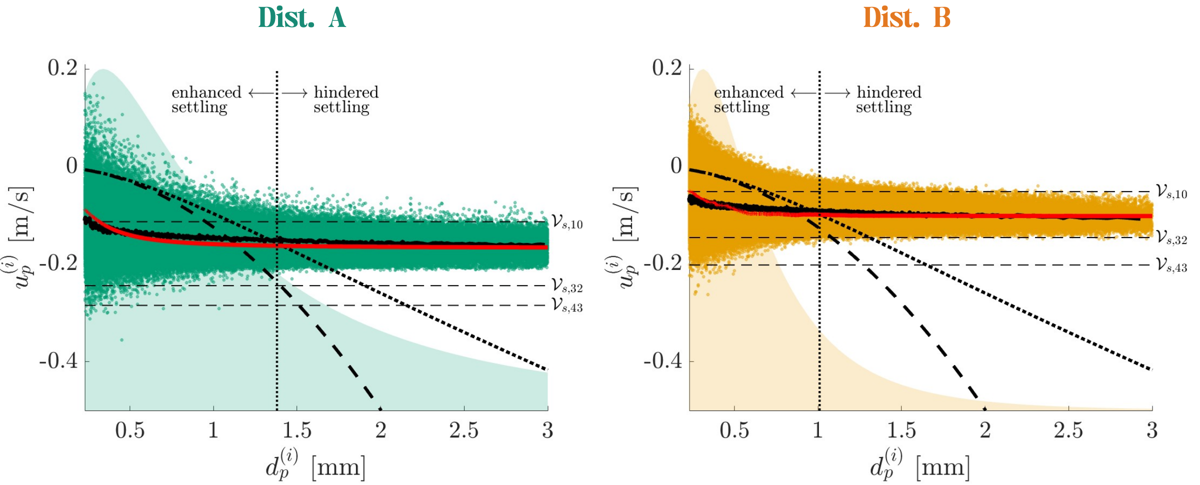

$\langle \alpha_p \rangle = 0.10$ $\langle \alpha_p \rangle = 0.10$

Key take-aways from this work

In this work, we made the following observations

- Large particles are most likely to generate clusters
- Cluster composition changes depending on polydispersity properties
- Smaller particles experience *enhanced* settling, and larger particles experience *hindered* settling.

and we made the following contributions

- The use of 'surface loading', $\mathcal{S}$ for predicting degree of heterogeneity and mean settling velocity for mono- and polydisperse assemblies.
- An improved model for C_D that captures enhanced settling for small particles and hindered settling for large particles.

Thank you!

Natural Environment Research Council

We acknowledge the support provided by NSF (2346972), NASA MSGC (80NSSC20M0124) and a NERC Independent Research Fellowship (NE/V014242/1).