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Effect of instantaneous local solid volume fraction on unsteady drag forces in freely evolving particle suspensions

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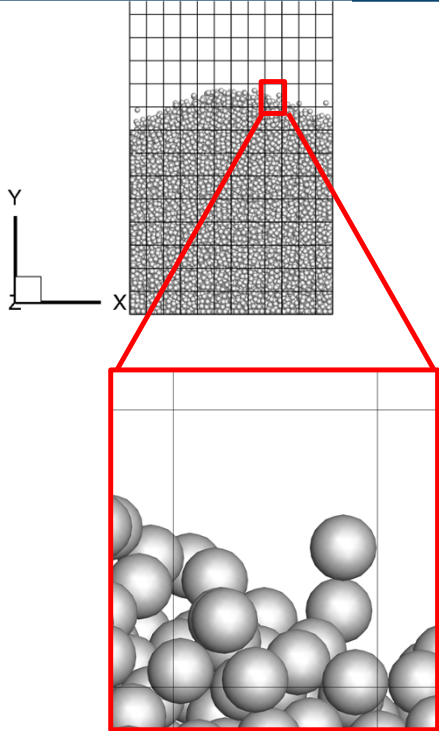
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Outline

- Motivation and Objectives
- Particle Resolved Simulations
- Results
- Conclusions

Motivation

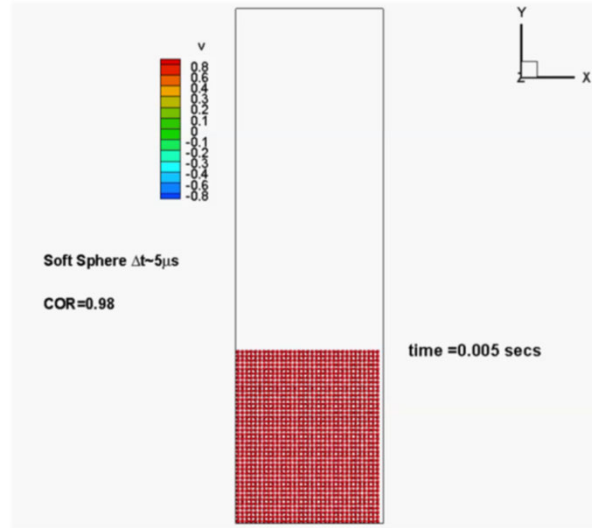
- In Euler-Lagrange simulations, particles are approximated as point masses on a grid spacing that is 3~5 times larger than the particle diameter



- Drag force correlation is essential in modeling interphase momentum exchange

- The Re-number and solid fraction by default are only available on the scale of the grid.

- Can we improve drag force predictions in point particle methods by using more precise information about the state of individual particles?

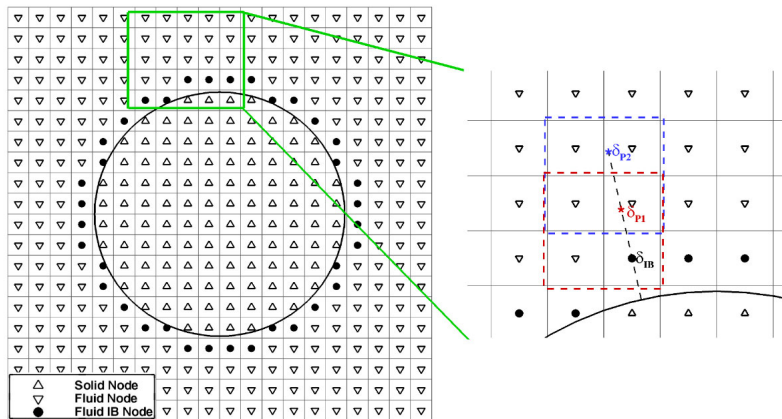


- CFD-DEM simulation of Muller's fluidized bed experiment (2009)

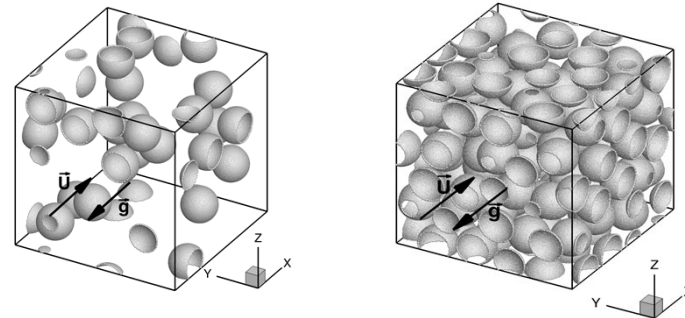
Author	Drag correlation
Di Felice (1994)	$F_d = F_{d0} \varepsilon^{-\chi}$ (ε : void fraction, equals to $(1 - \varphi)$), $\chi = 3.7 - 0.65 \exp\left[-\frac{(1.5 - \log Re)^2}{2}\right]$.
Tavanashad et al. (2021)	$F_d = F_{iso} \cdot (78.96\varphi^3 - 18.63\varphi^2 + 9.845\varphi + 1)^n$ $F_{iso} = 1 + 0.15Re^{0.687}$ $\begin{cases} n = 1, & \rho_s/\rho_f \leq 10 \\ \frac{1.05 - n}{n - 0.9} = 4.3 \times 10^{-4} Re^{2.361} & \rho_s/\rho_f = 100 \end{cases}$

Particle Resolved Simulations

- Study adopts Immersed Boundary Method (IBM) to perform Particle Resolved Simulations (PRS) for **freely evolving spherical particle suspensions**



- Simulations are performed within domain of $5d_p \times 5d_p \times 5d_p$ with d_p being the particle diameter



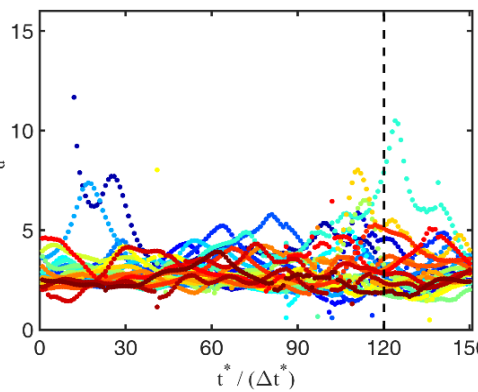
- The simulations cover:
 - **Particle-to-fluid density ratios ($\frac{\rho_s}{\rho_f}$) of 2, 10 and 100;**
 - **Solid volume fraction (ϕ) between 0.1 and 0.4;**
 - **Reynolds number (Re) from 10 to 300.**

Cao Z, Tafti DK. "Alternate method for resolving particle collisions in PRS of freely evolving particle suspensions using IBM". *International Journal of Multiphase Flow*. 2024 May 10:104862.
<https://doi.org/10.1016/j.ijmultiphaseflow.2024.104862>

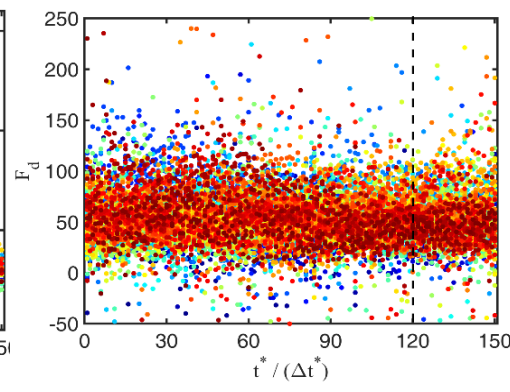
Particle Resolved Simulation Results

- Simulated time-development of individual particle drag forces

- Time development of individual particle drag forces in two suspensions



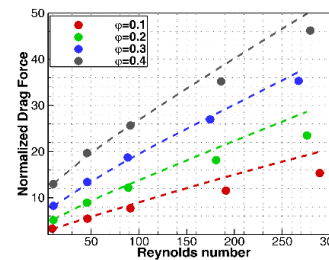
(a) $\frac{\rho_s}{\rho_f} = 2, Re=10, \varphi = 0.1$



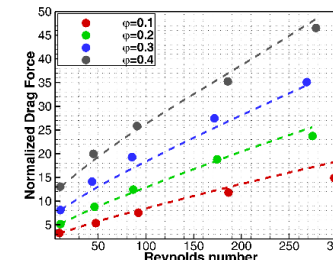
(b) $\frac{\rho_s}{\rho_f} = 2, Re=300, \varphi = 0.4$

- The PRS-derived suspension-mean drag forces are compared with Tavanashad et al. (2021) drag correlation proposed for freely evolving sphere suspensions

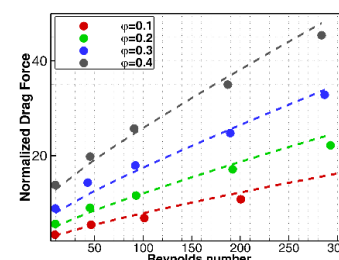
Author	Drag correlation
Tavanashad et al. (2021)	$F_d = F_{iso} \cdot (78.96\varphi^3 - 18.63\varphi^2 + 9.845\varphi + 1)^n$ $F_{iso} = 1 + 0.15Re^{0.687}$
	$\begin{cases} n = 1, & \rho_s/\rho_f \leq 10 \\ \frac{1.05 - n}{n - 0.9} = 4.3 \times 10^{-4} Re^{2.361} & \rho_s/\rho_f = 100 \end{cases}$



(a) $\frac{\rho_s}{\rho_f} = 2$



(b) $\frac{\rho_s}{\rho_f} = 10$



(c) $\frac{\rho_s}{\rho_f} = 100$

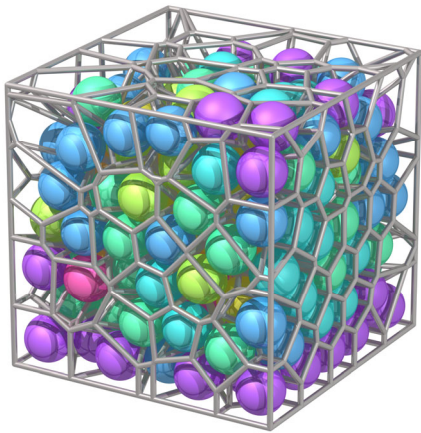
Definition of local solid volume fraction (φ_{loc})

- Calculate the volume of Voronoi tessellation for each particle in the suspension at each instant, defined as V_{vor}

- The local solid volume fraction is defined as:

$$\varphi_v = \frac{V_p}{V_{vor}} = \varphi_{loc}$$

- With V_p being the particle volume



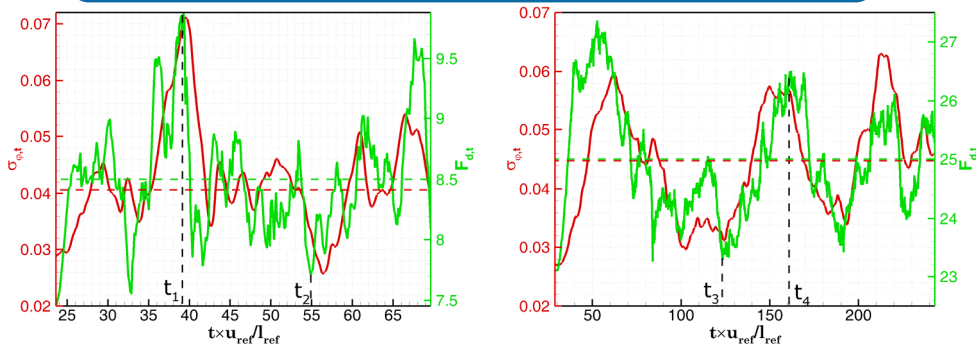
Snapshot of the Voronoi tessellations in suspensions of particles (*adapted from Voro++, n.d.*).

- **Periodic boundary conditions is accounted for in calculating V_{vor}**

Effect of suspension heterogeneity on drag force

- Denoting instantaneous individual particle drag force as $F_{d,i,t}$, i is the particle ID in the suspension and t is the time instant
- **Suspension-averaged instantaneous drag force** can be defined as:
 - $\bar{F}_{d,t} = \frac{1}{N} \sum_{i=1}^N F_{d,i,t}$ — N is the total number of particles in the suspension
 - Quantify **dispersion of instantaneous φ_{loc}** distribution among all particles in the suspension using standard deviation ($\sigma_{\varphi_{v,t}}$)

- $\bar{F}_{d,t}$ is observed to be positively correlated with $\sigma_{\varphi_{v,t}}$



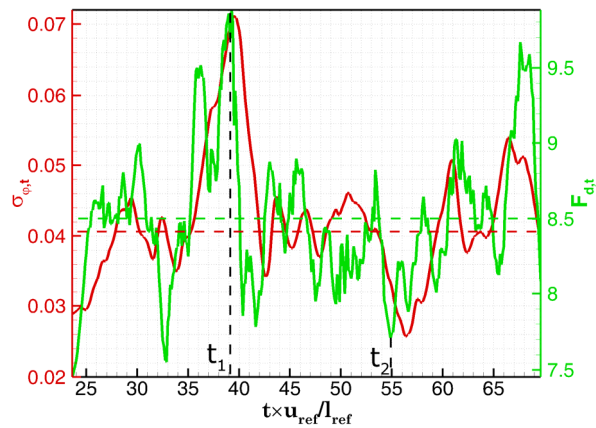
(a) Results at $\varphi = 0.2$, $Re = 50$, $\frac{\rho_s}{\rho_f} = 2$

(b) Results at $\varphi = 0.3$, $Re = 200$, $\frac{\rho_s}{\rho_f} = 100$

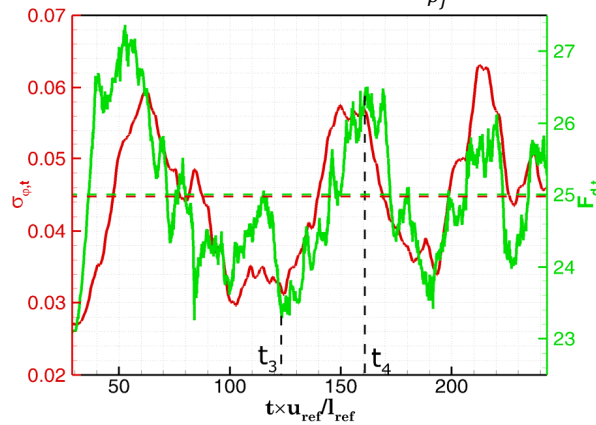
$\rho_s/\rho_f = 2$	Re = 10	-0.03	0.03	0.07	0.07
	Re = 50	0.20	0.46	0.50	0.44
	Re = 100	0.24	0.56	0.72	0.69
	Re = 200	0.49	0.64	0.77	0.73
	Re = 300	0.33	0.61	0.66	0.48
$\rho_s/\rho_f = 10$	Re = 10	0.46	0.20	0.33	0.34
	Re = 50	0.37	0.55	0.52	0.67
	Re = 100	0.16	0.66	0.75	0.89
	Re = 200	0.37	0.70	0.80	0.89
	Re = 300	0.17	0.43	0.76	0.65
$\rho_s/\rho_f = 100$	Re = 10	0.40	0.65	0.42	-0.02
	Re = 50	0.24	0.80	0.82	0.85
	Re = 100	0.03	0.74	0.61	0.84
	Re = 200	-0.40	0.66	0.69	0.62
	Re = 300	-0.05	0.58	0.53	0.14
		$\varphi = 0.1$	$\varphi = 0.2$	$\varphi = 0.3$	$\varphi = 0.4$

- Pearson correlation coefficient between $\bar{F}_{d,t}$ and $\sigma_{\varphi_{v,t}}$ at different conditions
- Significant positive correlation exists at $Re \geq 50$, $\varphi \geq 0.2$

Effect of suspension heterogeneity on drag force.....more

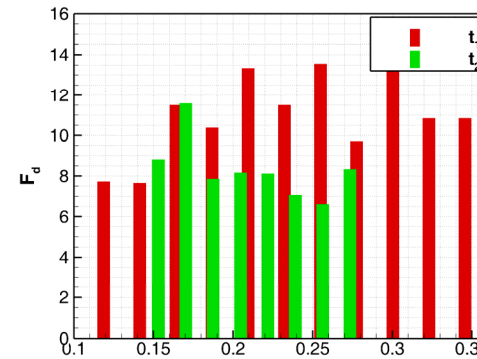
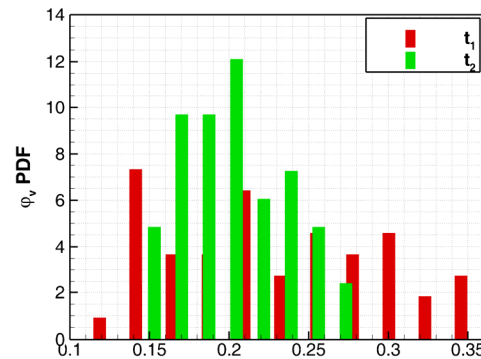


(a) Results at $\phi = 0.2, Re = 50, \frac{\rho_s}{\rho_f} = 2$



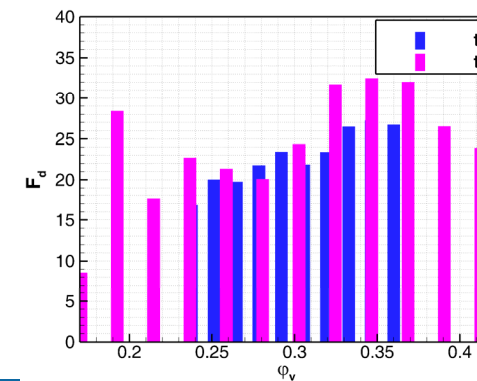
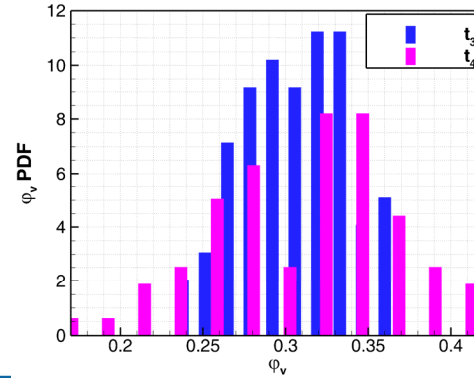
(b) Results at $\phi = 0.3, Re = 200, \frac{\rho_s}{\rho_f} = 100$

- PDF of ϕ_v at t_1, t_2, t_3 and t_4 are extracted together with particle drag forces as function of ϕ_v .



$$\frac{\rho_s}{\rho_f} = 2$$

$$\phi = 0.2, Re = 50$$



$$\frac{\rho_s}{\rho_f} = 100$$

$$\phi = 0.3, Re = 200$$

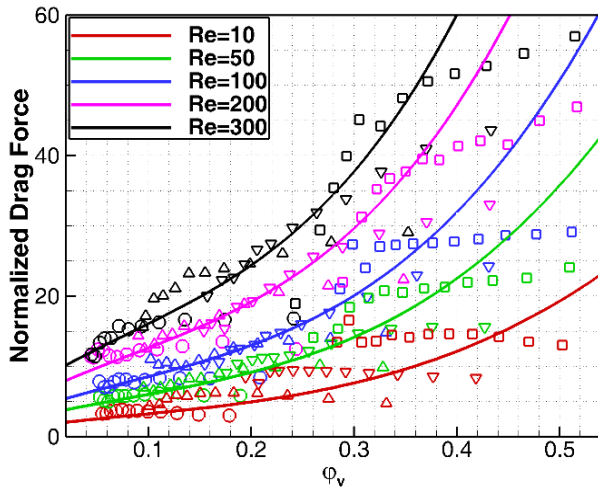
- Particles with $\phi_v > \phi$ contribute more than particles at $\phi_v < \phi$ to increase overall drag force

Can we use existing drag force correlations to include effect of φ_{loc} ?

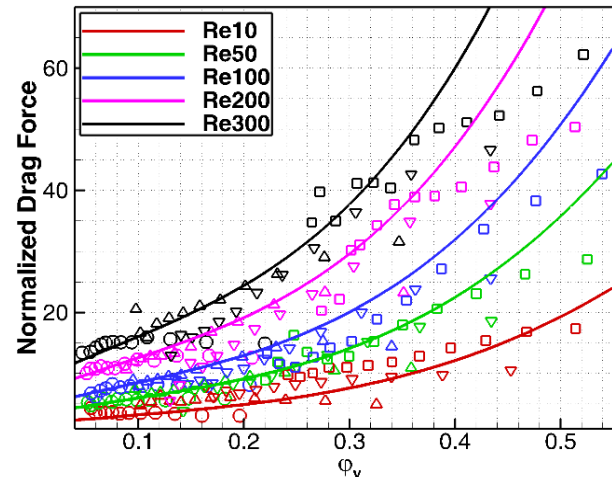
- Drag forces averaged within φ_v bins among all investigated conditions are plotted below with predictions using φ_v instead of φ in Tavanashad's drag force correlation

Author	Drag correlation
Tavanashad et al. (2021)	$F_d = F_{iso} \cdot (78.96\varphi_v^3 - .63\varphi_v^2 + 9.845\varphi_v + 1)^n$ $F_{iso} = 1 + 0.15Re^{0.687}$
	$\begin{cases} n = 1, & \rho_s/\rho_f \leq 10 \\ \frac{1.05 - n}{n - 0.9} = 4.3 \times 10^{-4} Re^{2.361} & \rho_s/\rho_f = 100 \end{cases}$

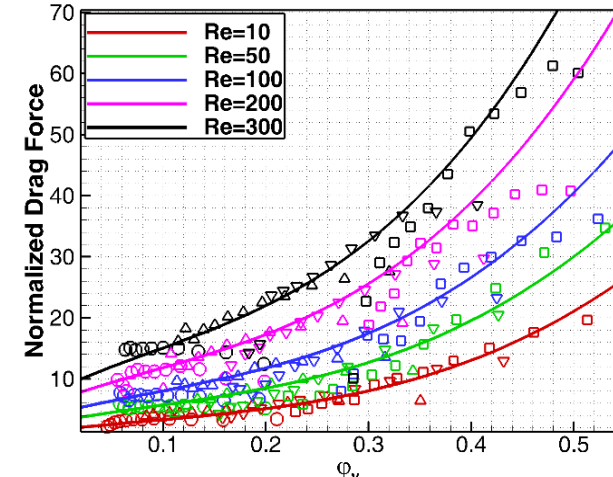
○ : $\varphi = 0.1$; △ : $\varphi = 0.2$; ▽ : $\varphi = 0.3$; □ : $\varphi = 0.4$



(a) $\frac{\rho_s}{\rho_f} = 2$



(b) $\frac{\rho_s}{\rho_f} = 10$



(c) $\frac{\rho_s}{\rho_f} = 100$

- Irrespective of φ for $\varphi_v < \varphi$, the effect of φ_v on drag force follows the same trend as that of φ
- As $\varphi_v > \varphi$, the increase in particle drag becomes less prominent and in most cases levels off

Use of modified solid fraction with Tavanashad drag force correlation

- With Reynolds number defined as:

$$Re = \frac{\rho_{ref}^* d_p^* (u_f^* - u_p^*) \varphi}{\mu_{ref}^*}$$

- Based on our observations, define modified local solid fraction, φ_1 :

$$\begin{cases} \varphi_1 = \varphi_v, & \varphi_v \leq \varphi \\ \varphi_1 = \varphi, & \varphi_v > \varphi \end{cases}$$

Comparison of use of φ_1 versus φ

- Mean Absolute Percentage Error (MAPE) defined as:

$$MAPE = \frac{1}{N \cdot M} \sum_{t=1}^M \sum_{i=1}^N \left| \frac{F_{d,i,t}^{PRS} - F_{d,i,t}^{corr}}{F_{d,i,t}^{PRS}} \right| \times 100\%$$

- N and M are total number of particles in the suspension and number of sampled time instances, respectively

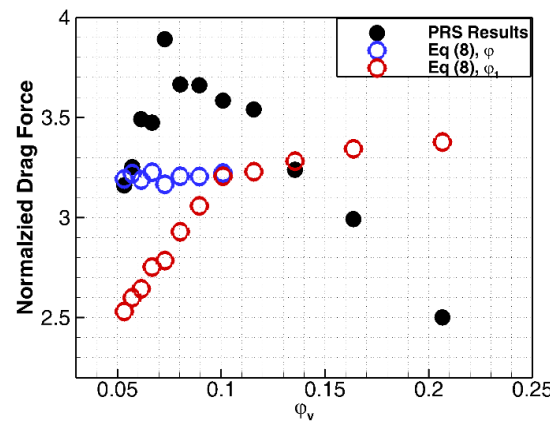
- The table below lists the decrease in MAPE when implementing φ_1 compared to φ in Tavanashad's drag force correlation

		$\varphi = 0.1$	$\varphi = 0.2$	$\varphi = 0.3$	$\varphi = 0.4$
$\rho_s/\rho_f = 2$	Re = 10	1.3%	1.6%	1.3%	0.8%
	Re = 50	2.3%	6.6%	15.2%	7.7%
	Re = 100	3.5%	7.1%	32.3%	7.5%
	Re = 200	3.3%	21.9%	16.3%	7.8%
	Re = 300	3.5%	6.1%	19.6%	11.9%
$\rho_s/\rho_f = 10$	Re = 10	0.6%	5.2%	7.6%	8.6%
	Re = 50	3.2%	8.4%	38.6%	19.6%
	Re = 100	5.1%	11.2%	39.5%	23.4%
	Re = 200	4.3%	17.0%	35.4%	18.2%
	Re = 300	2.8%	11.8%	33.7%	18.5%
$\rho_s/\rho_f = 100$	Re = 10	1.3%	6.5%	15.3%	23.1%
	Re = 50	1.2%	8.4%	37.1%	45.1%
	Re = 100	3.5%	9.7%	39.4%	18.0%
	Re = 200	13.4%	8.4%	11.0%	11.0%
	Re = 300	2.1%	4.9%	11.2%	23.6%

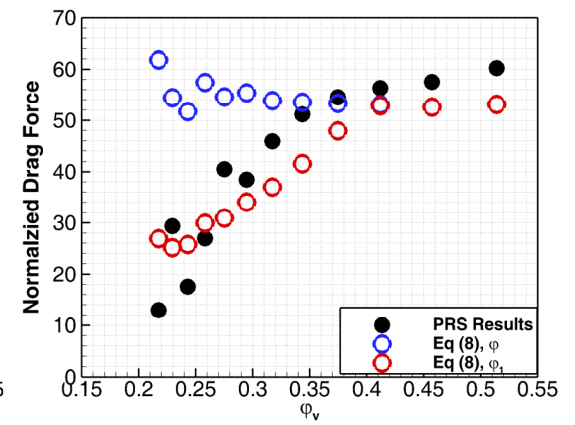
- The increase in accuracy becomes prominent when $Re \geq 50$, $\varphi \geq 0.3$, similar as the conditions when $\bar{F}_{d,t}$ and $\sigma_{\varphi_v,t}$ exhibit significant positive correlation

Drag force prediction using φ_1 versus φ in Tavanashad correlation

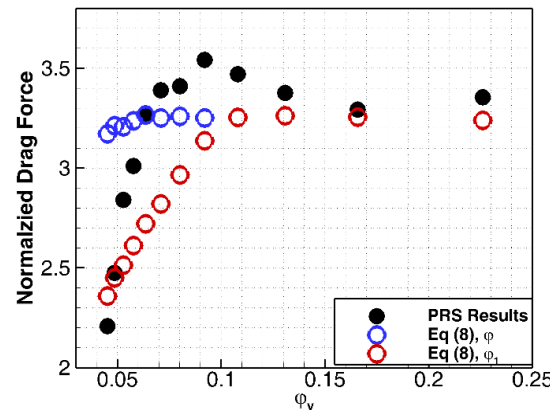
- The four left figures compare averaged drag forces within φ_v bins, derived from Tavanashad's drag correlation using φ_1 and φ , respectively, with the PRS data.
- Except for the case at $\frac{\rho_s}{\rho_f}=2, \varphi=0.1, Re=10$, $Re=10$, the variation in particle drag force with respect to φ_v is better captured when using φ_1 compared to φ



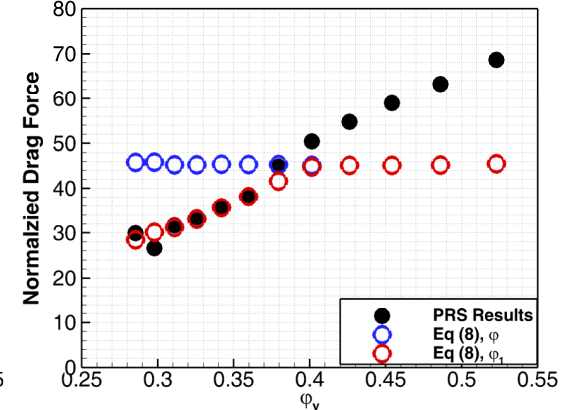
(a) $\frac{\rho_s}{\rho_f}=2, \varphi=0.1, Re=10$



(b) $\frac{\rho_s}{\rho_f}=2, \varphi=0.4, Re=300$



(c) $\frac{\rho_s}{\rho_f}=100, \varphi=0.1, Re=10$



(d) $\frac{\rho_s}{\rho_f}=100, \varphi=0.4, Re=300$

Drag force prediction using φ_1 versus φ in Huang correlation

- Huang et al. (2018) proposed a drag correlation for mobile particle suspensions, utilizing suspension averaged granular temperature (\bar{T}^*) to quantify the effect of particle mobility on drag force. \bar{T}^* is defined as:

$$\bar{T}^* = \frac{1}{T_n} \sum_{t=1}^{T_n} \left(\frac{1}{3N} \sum_{k=x,y,z} \sum_{i=1}^N \left(u_{p_{i,k}}^*(t) - \widehat{u}_{p_k}^*(t) \right)^2 \right)$$

- Where $u_{p_{i,k}}^*(t)$ is the instantaneous particle velocity along k -direction. A granular temperature based Reynolds number is derived as:

$$Re_T = \frac{\rho_{ref}^* \sqrt{\bar{T}^*} d_p^*}{\mu_{ref}^*}$$

- And Huang's drag correlation:

$$\bar{F}_d = \bar{F}_{stat} + 4.01 \frac{(1.93\varphi^2 + 0.25\varphi + 0.66)}{(1-\varphi)^{0.1}} \cdot \frac{Re_T^{1.49}}{Re^{0.8+100}}$$

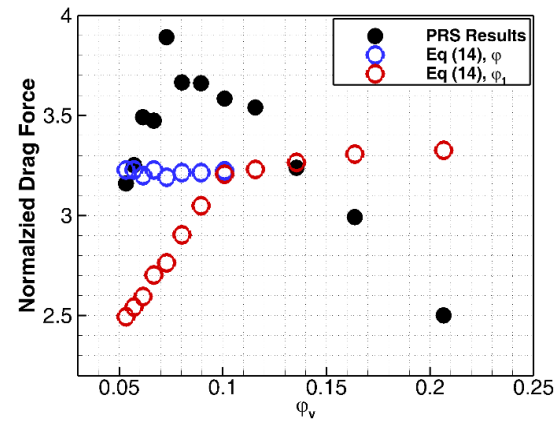
- Table on the left illustrates the decrease in **MAPE** when implementing φ_1 compared to φ in Huang's drag force correlation

$\rho_s/\rho_f = 2$	Re = 10	1.2%	2.1%	2.0%	1.8%
	Re = 50	1.8%	6.3%	11.6%	4.5%
	Re = 100	4.2%	7.6%	24.9%	3.0%
	Re = 200	6.0%	24.9%	13.3%	4.6%
	Re = 300	7.5%	10.4%	17.6%	10.8%
$\rho_s/\rho_f = 10$	Re = 10	0.3%	6.0%	8.8%	10.9%
	Re = 50	2.3%	7.2%	30.8%	13.1%
	Re = 100	4.8%	10.2%	29.5%	15.6%
	Re = 200	5.6%	17.7%	26.5%	12.8%
	Re = 300	5.4%	13.7%	26.0%	12.6%
$\rho_s/\rho_f = 100$	Re = 10	0.6%	6.3%	14.8%	22.7%
	Re = 50	0.0%	8.8%	35.7%	44.0%
	Re = 100	3.5%	10.8%	37.3%	16.9%
	Re = 200	17.1%	11.1%	10.9%	9.8%
	Re = 300	4.4%	8.2%	11.8%	20.3%
		$\varphi = 0.1$	$\varphi = 0.2$	$\varphi = 0.3$	$\varphi = 0.4$

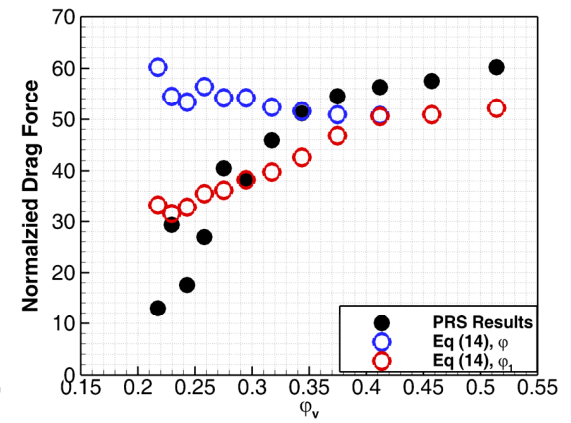
- The increase in accuracy becomes prominent when $Re \geq 50$, $\varphi \geq 0.3$, similar as the condition when implementing Tavanashad's drag correlation

Drag force prediction using φ_1 versus φ in Huang's correlation

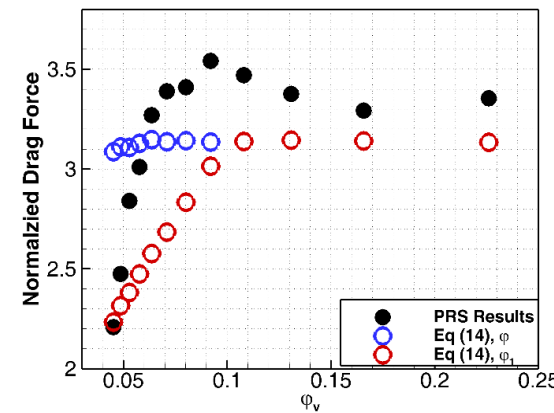
- Comparison of averaged drag forces within φ_v bins, derived from Huang's drag correlation using φ_1 and φ , respectively, with the PRS data, are plotted



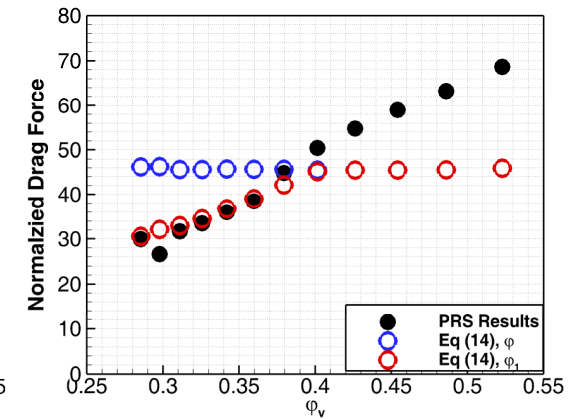
(a) $\frac{\mu_s}{\nu} = 2$, $\varphi = 0.1$, $Re = 10$



(b) $\frac{\mu_s}{\nu} = 2$, $\varphi = 0.4$, $Re = 300$



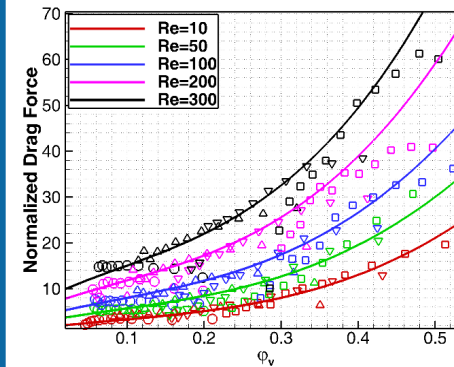
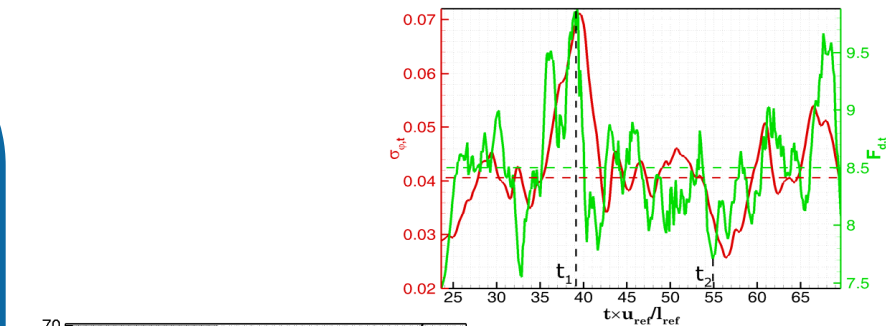
(c) $\frac{\rho_s}{\rho_f} = 100$, $\varphi = 0.1$, $Re = 10$



(d) $\frac{\rho_s}{\rho_f} = 100$, $\varphi = 0.4$, $Re = 300$

Summary and Conclusions

- Using particle resolved simulations of moving suspensions defined a local solid fraction for individual particles in the suspension as φ_v based on Voronoi tessellation
- Instantaneous variation of suspension averaged drag force $\bar{F}_{d,t}$ is observed to be positively correlated with the variation of φ_v measured by its standard deviation (σ_{φ_v})
- the dependency of individual particle drag force on φ_v when $\varphi_v \leq \varphi$ resembles the correlation between suspension-averaged drag force and φ
- Implementing $\varphi_1 \left(\begin{cases} \varphi_1 = \varphi_v, & \varphi_v \leq \varphi \\ \varphi_1 = \varphi, & \varphi_v > \varphi \end{cases} \right)$ in the drag correlations significantly improves drag prediction accuracy compared to using φ .



$\rho_s/\rho_f = 2$	Re = 10	1.3%	1.6%	1.3%	0.8%
	Re = 50	2.3%	6.6%	15.2%	7.7%
	Re = 100	3.5%	7.1%	32.3%	7.5%
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	Re = 100	3.5%	9.7%	39.4%	18.0%
	Re = 200	13.4%	8.4%	11.0%	11.0%
	Re = 300	2.1%	4.9%	11.2%	23.6%
		$\varphi = 0.1$	$\varphi = 0.2$	$\varphi = 0.3$	$\varphi = 0.4$