CoMFRE Multiphase Flow Research

Euler-Euler Model for Charge Transport in Fluidized Beds of Polyethylene Particles

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Industrial and experimental observations

Electrostatic effects of fluidization

- Charge accumulation in the bed and increase of electric potential
- Particle sticking on the walls of the fluidized bed
- Risk of fire due to large electric potential development

Potential consequences for polyethylene production

- Reduction of heat transfer from the reactor
- Formation of sheets of molten particles (sheeting)
- Detachment of sheets leading to inlet clogging and defluidization

Polyethylene particles deposited on fluidized bed wall (view from bottom of bed)

The discrete particle-wall and particle-particle charging models

Rate of change of particle charge due to collision with wall (Matsusaka and Masuda, 2003):

$$\frac{\mathrm{d}q}{\mathrm{d}\mathbf{n}_c} = k_c \varepsilon_0 \varepsilon_r \left[\frac{V_c}{z_0} \left(1 - \frac{q}{q_\infty} \right) + \mathbf{E}_q \cdot \mathbf{n} \right] S_w$$

Rate of change of particle charge due to collision with another particle of the same material but different size (Schein et al. (1992))

$$\frac{\mathrm{d}q_1}{\mathrm{d}\mathbf{n}_c} = k_c \varepsilon_0 \varepsilon_r \left[\frac{q_2}{\pi d_2^2 \varepsilon_0 \varepsilon_r} - \frac{q_1}{\pi d_1^2 \varepsilon_0 \varepsilon_r} + \mathbf{E}_q \cdot \mathbf{k} \right] S_{\boldsymbol{p}} = \left[-K_1 q_1 + K_2 q_2 + K_{eq} (\mathbf{E}_q \cdot \mathbf{k}) \right] v^{4/5}$$

where

- ε_0: permittivity of vacuum
- ε_r: relative permittivity of the material
- V_c: work function difference between contacting surfaces
- q_∞: saturation charge density
- k_c: charging efficiency
- z_0: critical gap
- $\mathbf{E}_q$: electric field at the point of contact

Hertzian model for the maximum contact area:

$$S_w = 1.364 d_{1,2}^2 v^{4/5} \left[\rho_s \frac{1-\nu}{E} \right]^{2/5}$$

$$S_{\boldsymbol{p}} = 1.364 d_{\mathrm{eq}}^2 v^{4/5} \left[\rho_s \frac{1-\nu}{E} \right]^{2/5}$$

where:

- $d_{1,2}$: particle diameter (s)
- d_{eq}: equivalent particle diameter (Hertz)
- E: Young's elastic modulus of particle material
- ν: Poisson ratio of particle material
- ρ_s: Particle density

Coupling of hydrodynamic and electrostatic models

Momentum equation of the particle phase

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \mathbf{U}_s) + \nabla \cdot (\alpha_s \rho_s \mathbf{U}_s \otimes \mathbf{U}_s) = \nabla \cdot \boldsymbol{\tau}_s - \alpha_s \nabla p - \nabla p_s + \alpha_s \rho_s \mathbf{g} + \mathbf{M}_{gs} + \mathbf{F}_q$$

$$\mathbf{F}_q = q \alpha_s \mathbf{E}_q$$ Electrostatic force

Poisson equation for electrical potential

$$\nabla \cdot (\varepsilon_0 \varepsilon_m \nabla \varphi_E) = \rho_q = q \alpha_s$$

$$\mathbf{E}_q = -\nabla \varphi_E$$ Electric field

Charge transport equation

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \langle q \rangle) + \nabla \cdot (\alpha_s \rho_s \langle q \rangle \mathbf{U}_s) + \nabla \cdot (\alpha_s \rho_s \langle \mathbf{C} q' \rangle) = m_p \mathbb{C}(q)$$

Charge and velocity covariance

Rate of change of charge due to collisions

From the kinetic theory of granular flows

Monodisperse modeling

Charge-velocity covariance (monodisperse)

Transport equation of charge-velocity $\langle \mathbf{c}q \rangle$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \langle \mathbf{c}q \rangle) + \nabla \cdot (\alpha_s \rho_s \langle \mathbf{c}\mathbf{c}q \rangle) = m_p \mathbb{C}(\mathbf{c}q) + \alpha_s \rho_s \langle \frac{\partial \mathbf{c}q}{\partial \mathbf{c}} \frac{\mathrm{d}\mathbf{c}}{\mathrm{dt}} \rangle + \alpha_s \rho_s \langle \frac{\partial \mathbf{c}q}{\partial q} \frac{\mathrm{dq}}{\mathrm{dt}} \rangle$$

Assumptions:

- $\langle \mathbf{c}q \rangle$ is a quasi-steady variable
- $\langle \mathbf{C}\mathbf{C}q' \rangle = 0$
- Divergence of terms containing $\mathbf{U}_s$ is negligible
- Gradients of $\alpha_s, \langle \mathbf{C}\mathbf{C} \rangle$ are negligible compared to gradients of $\langle q \rangle$ and electric potential

$$\langle \mathbf{C}q' \rangle = -\frac{1}{(1+e)\sqrt{\pi \Theta_s} + \left[\left(\frac{5}{7} - \frac{5}{12}(1+e)\right) 2^{14/5} \Gamma\left(\frac{12}{5}\right) \sqrt{\pi} K_1 {\Theta_s}^{9/10}\right]} \times \left[\left(\frac{\pi}{30}(1+e) + \frac{\pi}{6 g_0 \alpha_s}\right) d_p \Theta_s \nabla \langle q \rangle - \frac{\pi d_p}{6 g_0 \alpha_s} \langle \frac{\mathbf{F}}{m_p} \rangle \langle q \rangle\right.$$

Charge transport equation (monodisperse)

Transport equation of charge

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \langle q \rangle) + \nabla \cdot (\alpha_s \rho_s \langle q \rangle \mathbf{U}_s) + \nabla \cdot \mathbf{q}_q = 0$$

Assumptions:

- Same as for charge−velocity correlation
- $f^{2} = g_0 f_{p1} f_{p2} \left(1 + \frac{\mathrm{d_p}}{2} (\mathbf{k} \cdot \nabla) \ln \frac{f_{p2}}{f_{p1}}\right) =$ $g_0 f_{p1} f_{p2} \left[1 + \frac{\mathrm{d_p}}{2} \left(\frac{1}{2Q^4} q_{12} (q_2 + q_1)(\mathbf{k} \cdot \nabla \langle q' q' \rangle) - \right.\right.$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \langle q \rangle) + \nabla \cdot (\alpha_s \rho_s \langle q \rangle \mathbf{U}_s) + \nabla \cdot \left\{ \alpha_s \rho_s \left[\left(1 + 2^{\frac{9}{5}} \Gamma\left(\frac{19}{10}\right) \frac{60 K_1 g_0 \alpha_s {\Theta_s}^{\frac{2}{5}}}{19\sqrt{\pi}} \right) \langle \mathbf{C} q' \rangle + \left(\frac{5}{9} 2^{9/5} \Gamma\left(\frac{12}{5}\right) \frac{1}{\sqrt{\pi}} K_{eq} g_0 \alpha_s {\Theta_s}^{\frac{9}{10}} \right) \mathbf{E}_q \right.\right.$$

Particle-wall charge flux

Derived consistently with the Johnson and Jackson (1987) boundary condition

Rate of change of charge due to collisions with the wall is given as:

$$\mathbb{C}_w(q) = -g_0(\alpha)\int_{\mathbf{c}\cdot\mathbf{n}<0} (q' - q) f(\mathbf{c})\mathbf{c}\cdot\mathbf{n}d\mathbf{c}$$

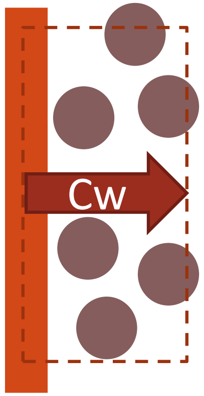
Using the discrete charging model of Matsusaka and Masuda (2003):

$$\frac{dq}{d\mathbf{n}_c} = q' - q$$

A Maxwellian velocity distribution is assumed (Johnson and Jackson, 1987).

Calculating the collision integral gives

$$\begin{aligned}\mathbb{C}_w(q) &= \frac{5}{7} g_0(\alpha) k_c k_s \varepsilon_0 \varepsilon_r N \\ &\times \frac{1}{2^{1/10}\sqrt{\pi}}\Gamma\left(\frac{12}{5}\right)\Theta_s^{9/10} \\ &\times \left[\frac{V_c}{z_0}\left(1 - \frac{q}{q_\infty}\right) + \mathbf{E}_q\cdot\mathbf{n}\right] = k_w\left[\frac{V_c}{z_0}\left(1 - \frac{q}{q_\infty}\right) + \mathbf{E}_q\cdot\mathbf{n}\right]\end{aligned}$$



Average flux of charge due to collisions

Noting that: $\mathbb{C}_w = -\mathbf{q}_q\cdot\mathbf{n}$

$$q_w = q_\infty\left[1 + \frac{z_0}{V_c}\left(\mathbf{E}_q + \frac{\mathbf{q}_q}{k_w}\right)\cdot\mathbf{n}\right]$$

Experimental test case [1]

Phase 1: Fluidization

- The bed is fluidized for 60 minutes with an inlet velocity of 150% of the minimum fluidization velocity (bubbling flow regime)

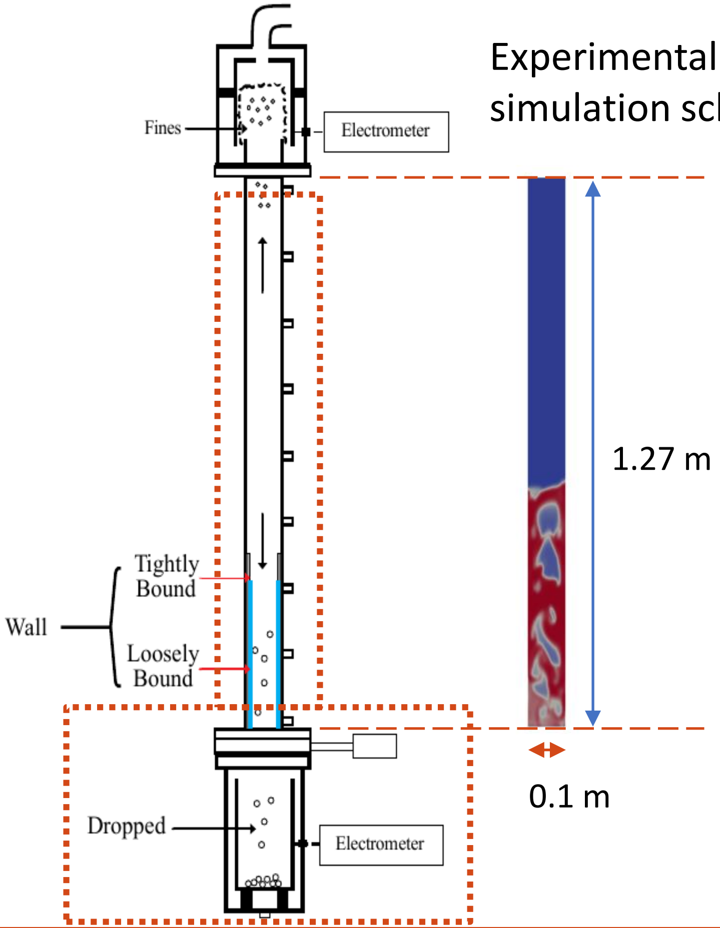
Phase 2: Settling and Dropping

- Air is stopped, and particles are allowed to settle
- The knife gate valve is opened to allow particles to drop
- Charge distribution of dropped particles is measured

Phase 3: Tapping

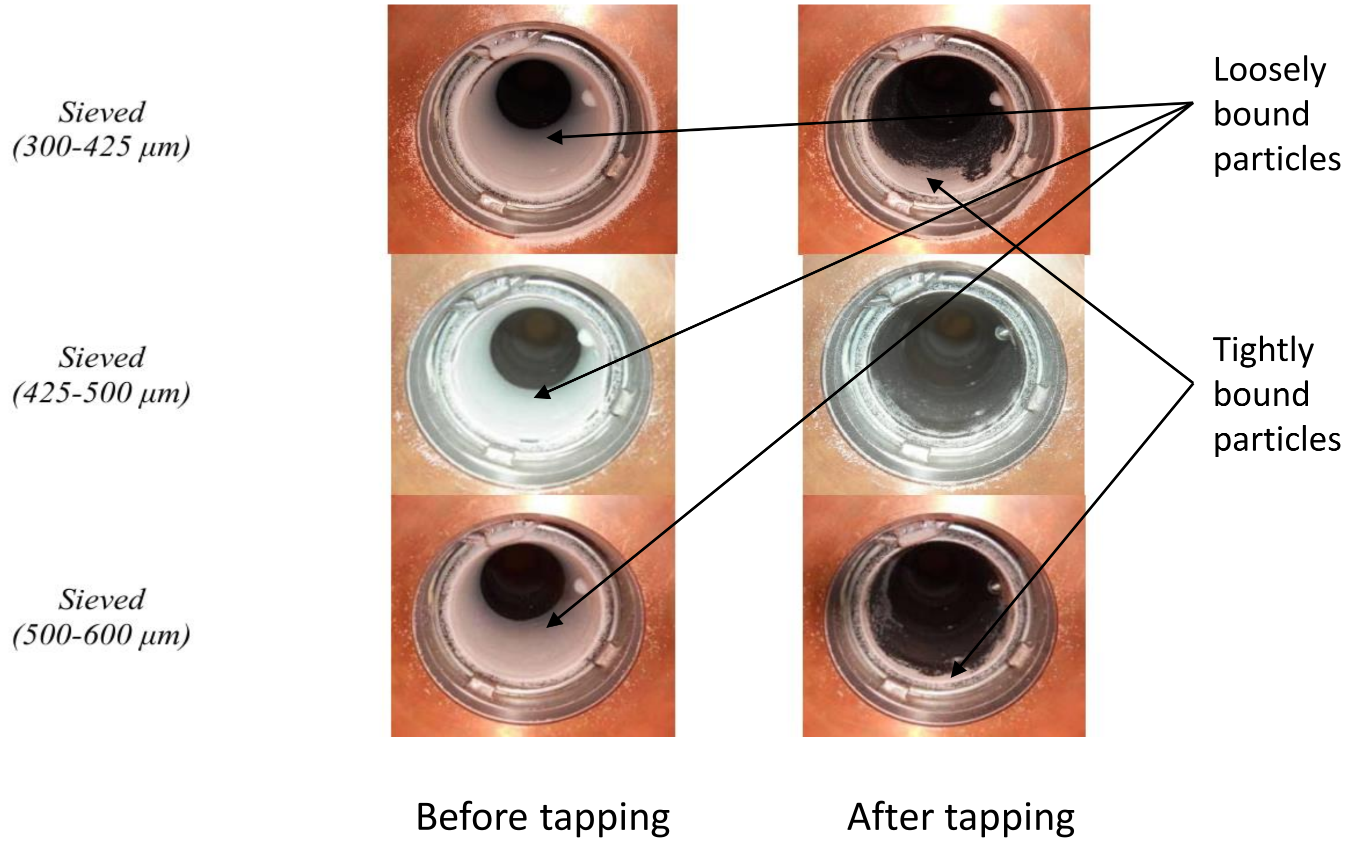
- The remaining particles clinging on the wall are categorized into two types based on their sticking intensity
- The column wall is tapped, and the loosely bound particles drop and collected
- The charge and size distributions of these particles are also recorded

Experimental setup with simulation schematic



Experimental test case [2]

- **PE fouling the inner wall of the fluidized bed. Images taken from the bottom of the fluidization column**



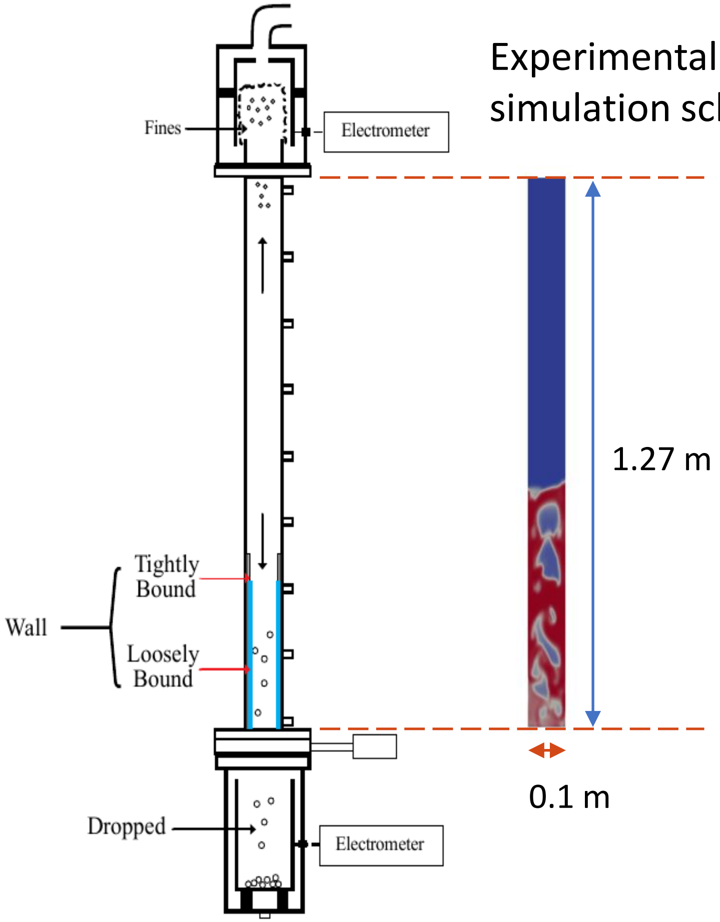
Simulation case

Phase 1: Fluidization

- The bed is fluidized with an inlet velocity of 150% of the minimum fluidization velocity corresponding to different particle size ranges till steady state is reached

Phase 2: Settling

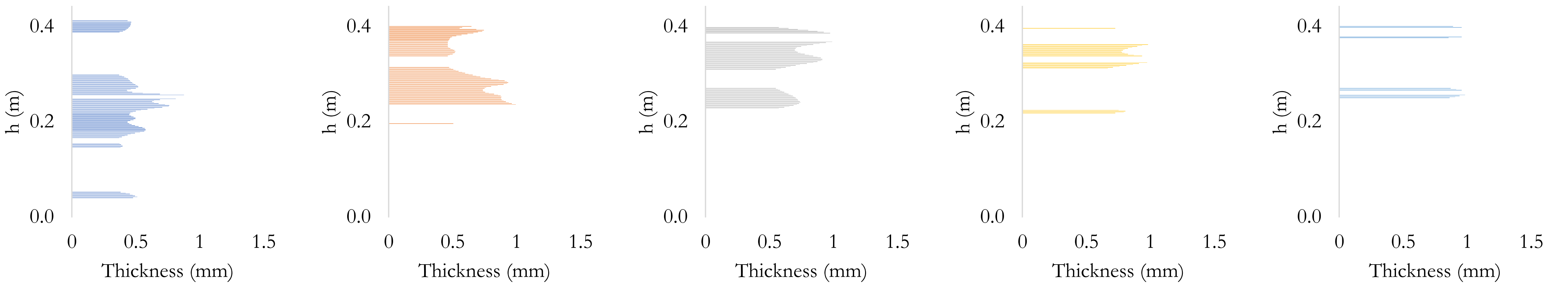
- Air flow is stopped, and particles are allowed to settle



Experimental setup with simulation schematic

Simulation results [2]

Thickness of wall particle layer after settling (based on friction-weight force balance)



362 μm

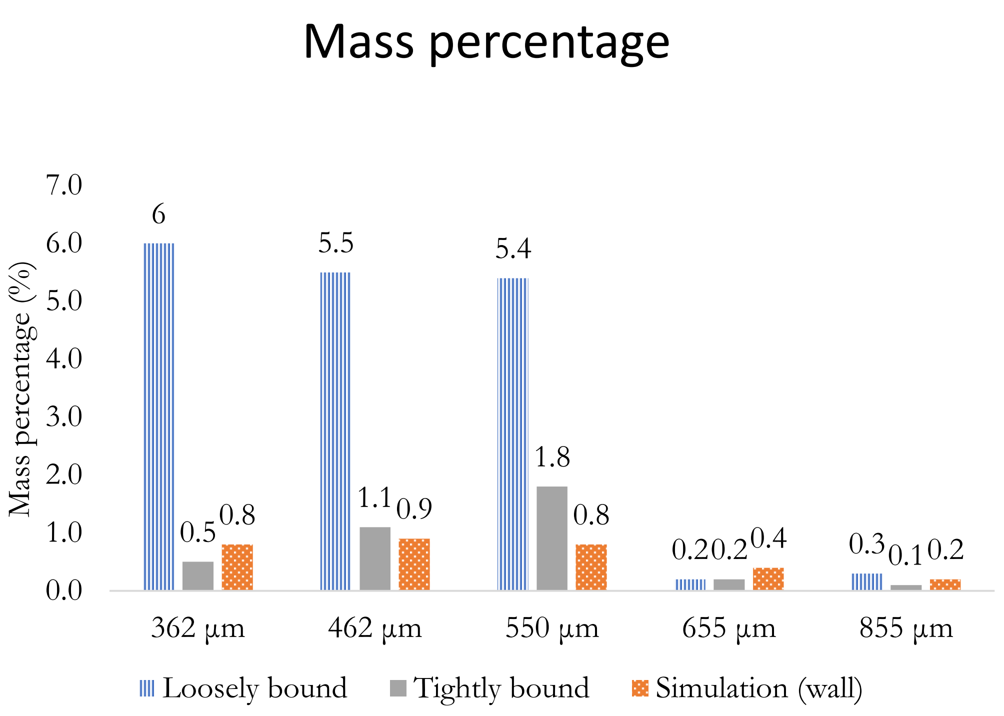
462 μm

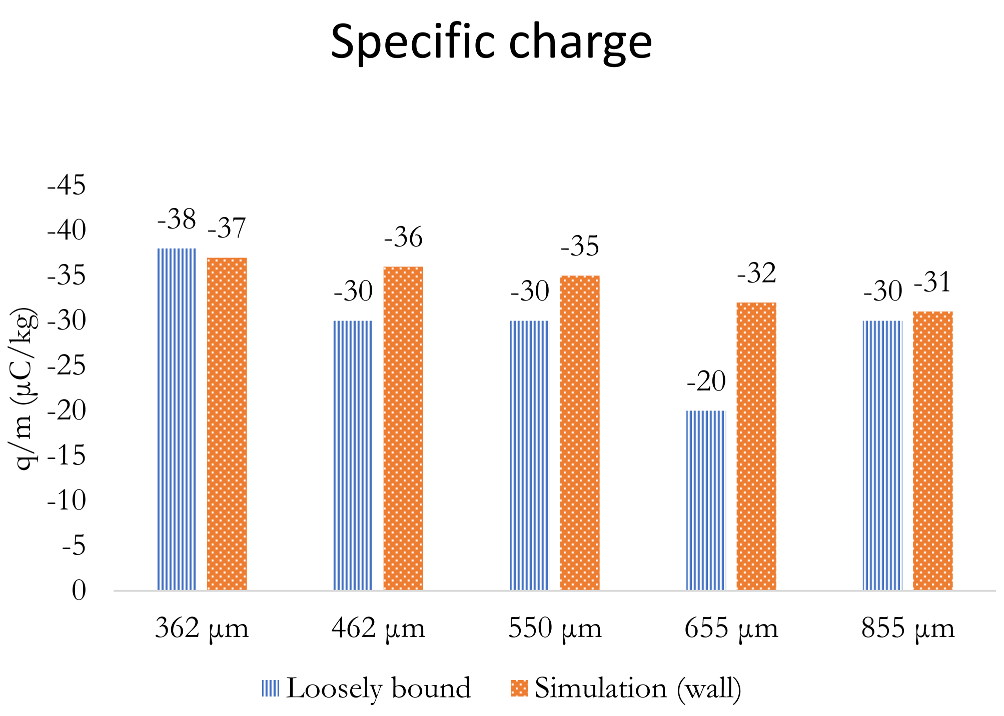
550 μm

655 μm

855 μm

Simulation results [3]





Bidisperse modeling

0-D FORMULATION

Assumptions

- The particle phases have **constant fluctuation velocity** and **no mean phase velocity**
- All **divergence** terms and **gradients** of all variables except electric potential is **negligible**
- The electric field strength is assumed constant (the **Laplacian** of electric potential is **neglected**)
- Other assumptions used in the monodisperse case are also considered for the formulation

Mean phase charge (bidisperse)

$$0 = g_{12} d_{12}^2 N_1 N_2 \left[\frac{5}{7} \Gamma\left(\frac{12}{5}\right) \sqrt{\pi} {\Theta_{12}}^{9/10} 2^{19/10} \right] \left(-K_1 \langle q_1 \rangle + K_2 \langle q_2 \rangle\right)$$

↓

$$\langle q_2 \rangle = \frac{K_1}{K_2} \langle q_1 \rangle$$

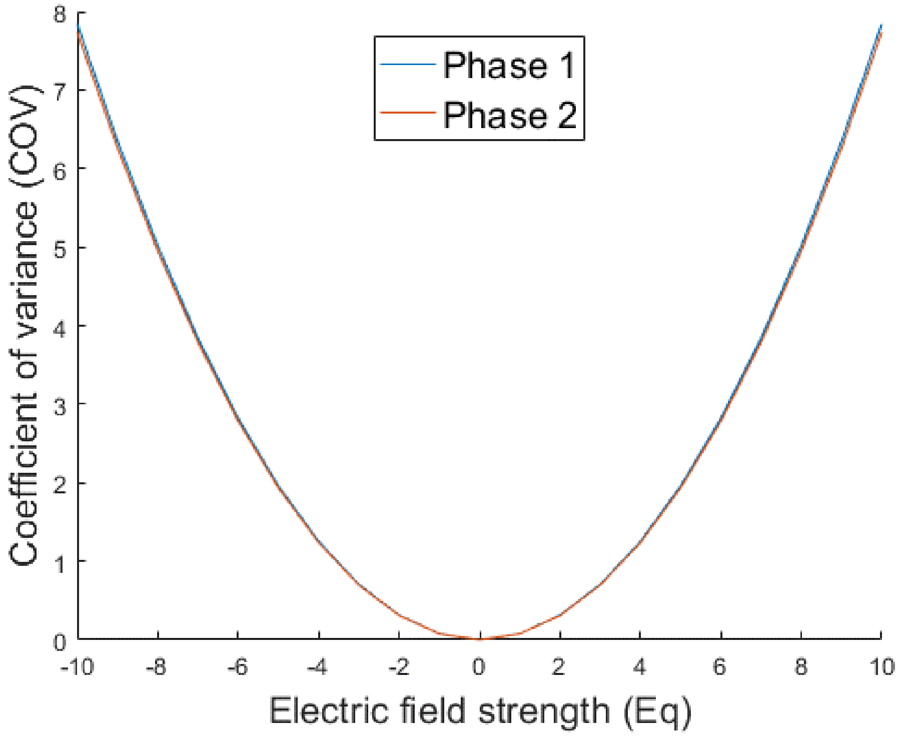
Charge-velocity covariance (bidisperse)

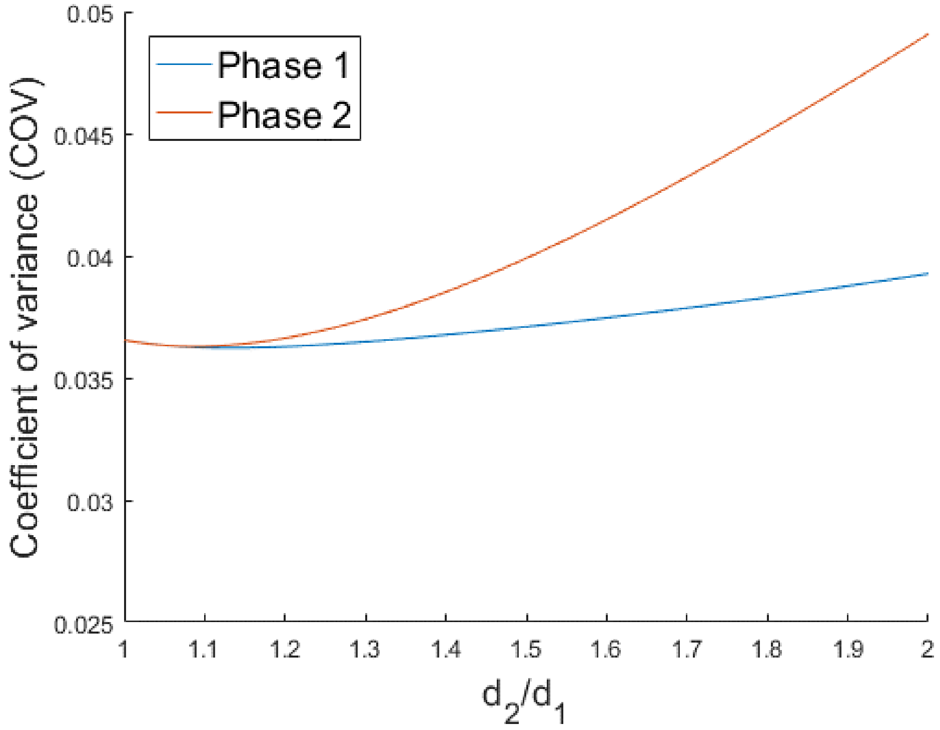
$$\mathbf{0} = m_1 M_2 g_{12} d_{12}^2 N_1 N_2 \left[\left\{ (1+e)\sqrt{\pi\Theta_{12}} + \frac{5}{7} 2^{19/10} \Gamma\left(\frac{12}{5}\right) \sqrt{\pi} \frac{K_1}{M_2} K_1 {\Theta_{12}}^{9/10} \right\} \langle \mathbf{C}_1 {q'}_1 \rangle + \frac{5}{12} (1+e) 2^{19/10} \Gamma\left(\frac{12}{5}\right) \sqrt{\pi} {\Theta_{12}}^{9/10} \left(K_1 \langle \mathbf{C}_1 {q'}_1 \rangle + K_2 \langle \mathbf{C}_2 {q'}_2 \rangle \right) \right.$$

Charge variance (bidisperse)

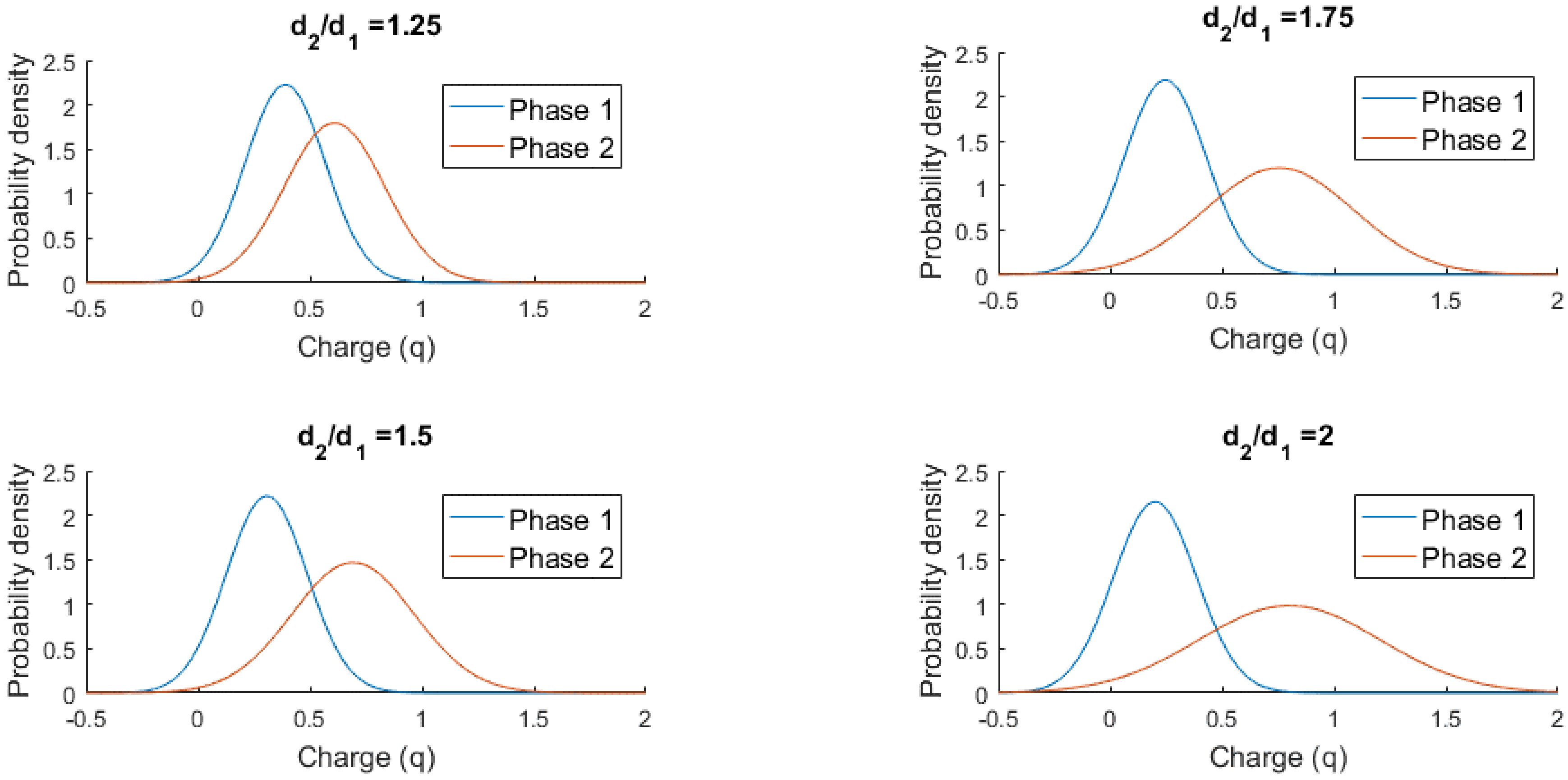
$$0$$
$$= g_{12} d_{12}^2 N_1 N_2 \left[-\frac{5}{7} \Gamma\left(\frac{12}{5}\right) \sqrt{\pi} {\Theta_{12}}^{9/10} 2^{23/10} K_1 \langle {q'}_1 {q'}_1 \rangle \right.$$
$$+ \frac{5}{9} \Gamma\left(\frac{14}{5}\right) \sqrt{\pi} {\Theta_{12}}^{13/10} 2^{23/10} \left(K_1^2 \langle {q'}_1 {q'}_1 \rangle + K_2^2 \langle {q'}_2 {q'}_2 \rangle \right) - \frac{5}{19} \Gamma\left(\frac{19}{10}\right) \sqrt{\pi} {\Theta_{12}}^{2/5} 2^{17/5} K_{\mathrm{eq}} \mathbf{E}_q \cdot \langle \mathbf{C}_1 {q'}_1 \rangle$$

Variation of charge COV with diameter ratio and electric field strength

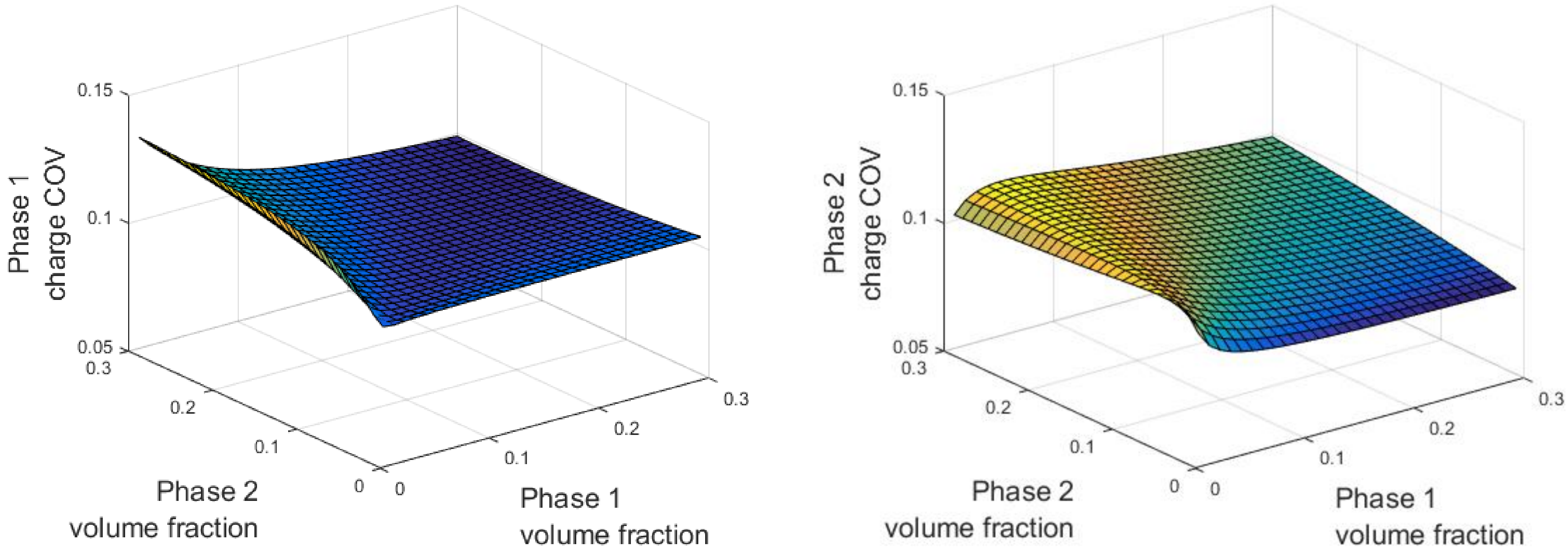




Charge distribution between two phases for a given total quantity of charge and varying diameter ratio



Variation of charge COV with phase volume fractions for diameter ratio of 1.2 and electric field strength of 1.0



Summary

A charge transport model for the **monodisperse** case incorporating **self-diffusion** was developed and implemented in **OpenFOAM** in conjunction with the **two-fluid Eulerian** model

Model was validated against experimental results by comparing **specific charge** and **mass percentage** of particles sticking to the wall

In agreement with the experiment, the simulation predicted a **lower proclivity** of sticking to the wall with **increasing particle size**. The specific charge and mass fraction values in simulation agreed reasonably with experiments

A charge transport model for the **bidisperse case** was derived and a 0-D formulation of the same is discussed - a simple case is set up with non-dimensional values to test the effect on charge distribution due to variations in parameters

Future work

Implement the **bidisperse model** in conjunction with the **polydisperse Eulerian model** in **OpenFOAM**

Validate against experimental results

Use the model to simulate **industrial scale** fluidization columns

Vary parameters and reactor design to suggest methods for **mitigating particle sheeting**

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Questions?