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Behrad Esgandari, Zahra Aminigarakani, Bradley Paul Ladewig, Simon Schneiderbauer

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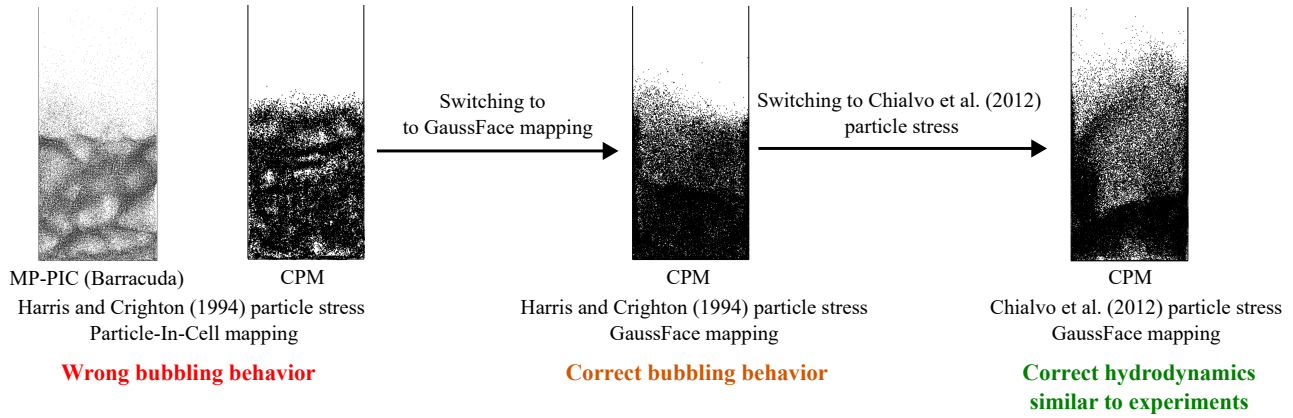
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1 Graphical Abstract

Instantaneous particle distribution

2 Highlights

- 3 • A face-interpolation-based CPM implementation is introduced.
- 4 • CPM agrees better with CFD-DEM and experiments than MP-PIC.
- 5 • Shear stress and advanced mapping improve CPM predictions compared to MP-PIC.
- 6 • CPM predicts shorter mixing times than CFD-DEM.

Application of the Continuum Particle Method to bubbling-fluidized and spout-fluidized beds

Behrad Esgandari^{a,*}, Zahra Aminigarakani^b, Bradley Paul Ladewig^b, Simon Schneiderbauer^{a,*}

^a*Department of Particulate Flow Modelling, Johannes Kepler University, Altenbergerstr.
69, 4040, Linz, Austria*

^b*Paul Wurth Chair, Department of Engineering, Faculty of Science, Technology and Medicine, University of
Luxembourg, Belval Campus, 2, place de l'Université, L-4365, Esch-sur-Alzette, Luxembourg*

Abstract

We develop a new implementation of the Continuum Particle Method (CPM) introduced by Verma and Padding (2020), a novel approach to multiphase particle-in-cell (MP-PIC) simulations, based on a face interpolation method that aims to improve robustness and accuracy. We present a comprehensive comparison of CPM, MP-PIC, and computational fluid dynamics coupled with the discrete element method (CFD-DEM) against experimental data from the literature for fluidized and spout-fluidized systems. We evaluate the methods using two drag models and show that CPM agrees better with both experiments and CFD-DEM. We demonstrate that the unsatisfactory performance of MP-PIC does not primarily arise from the selected drag model. Instead, it results from the simplified particle stress model, which depends only on the local particle volume fraction. This model accounts only for isotropic particle pressure and neglects viscous and frictional particle stresses, thereby missing key resistance mechanisms associated with shear and elongational deformation in dense particle regions. We also examine the role of smoothing in CPM by varying the characteristic smoothing length applied to particle fields. We show that smoothing strongly affects the predicted flow behavior and that the optimal level of smoothing depends on the operating flow regime. Finally, we assess particle mixing and find that CPM predicts faster mixing than CFD-DEM under the investigated conditions. Overall, we show that CPM offers a promising and computationally efficient alternative for simulating dense gas-solid flows while retaining improved agreement with benchmark numerical and experimental results.

Keywords: Continuum particle method (CPM), CFD-DEM, MP-PIC, Fluidized bed, Particle field smoothing

*Corresponding author at: Department of Particulate Flow Modelling, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Email addresses: `esgandari.behrad@gmail.com` (Behrad Esgandari), `simon.schneiderbauer@jku.at` (Simon Schneiderbauer)

1. Introduction

The examples of fluid-particle flows can be seen all around us from environmental flows such as sediment transport (Rahimi-Larki et al., 2026), contaminant transport in ground waters (Miller et al., 1998), and volcanic eruption (Lube et al., 2020), to many industrial applications, including, pneumatic conveying (Erken et al., 2024), fluidized beds (Schneiderbauer, 2018; Esgandari et al., 2021), spouted beds (Golshan et al., 2017; Hoorijani et al., 2023; Esgandari et al., 2023; Zand and Saidi, 2022), and risers (Capecelatro et al., 2014; Shaffer et al., 2013). The presence of the particle-phase in these flows leads to a broad range of length scales. These scales range from boundary layers and wakes on the surface of particles (typically of the order of micrometers/millimeters) termed as microscale, to particle volume fraction variations such as bubbles and heterogeneous particle structures (i.e., clusters) occurring in scales larger than particle size and smaller than the size of the system termed as mesoscale. The largest particle-laden flow structures are dictated by the size of the actual system (meters or kilometers) termed as macroscale (Subramaniam and Balachandar, 2022).

The multi-scale nature of fluid-particle systems necessitates the need for a multi-scale modelling strategy capable of simulating the fluid-particle flows at various length and time scales with different levels of detail. Among the available multi-scale approaches, the TFM, MP-PIC method, and CFD-DEM are commonly used to simulate large systems. All of the mentioned approaches employ the locally-averaged Navier–Stokes equations to resolve the fluid phase on an Eulerian grid and utilize similar interphase closure models (i.e., drag and turbulence) to achieve two-way coupling between the fluid and particle phases. The key difference lies in their treatment of the particle phase: TFM models it as a continuum, while MP-PIC and CFD-DEM represent it as discrete phase. TFM employs kinetic theory of granular flows (KTGF) concept to describe particle-particle interactions. Meanwhile, in MP-PIC, particles are tracked in a Lagrangian framework, often using a parcel approach in which a single simulated particle represents many physical particles. Each parcel evolves according to Newton’s equations of motion. Instead of explicitly resolving individual particle–particle collisions, MP-PIC models their collective effects through particle stress closures like the one proposed by Harris and Crighton (1994) and Srivastava and Sundaresan (2003). The particle stress gradient is evaluated on the Eulerian grid and then is interpolated to the location of the particles. CFD-DEM considers discrete particles, tracking movement of individual particles using Newton’s equations of motion similar to MP-PIC, and captures particle-particle interactions with hard-sphere (Hoomans et al., 1996) or soft-sphere (Cundall and Strack, 1979) models.

For systems with very large particle numbers, CFD-DEM is often computationally prohibitive, and TFM or MP-PIC is therefore more commonly used. A key advantage of MP-PIC over TFM is that the solid-phase is represented by Lagrangian particles rather than a purely continuum description. This particle-based representation enables direct access to particle-scale statistics that are difficult to obtain with TFM. For example, MP-PIC can account for particle size distributions and facilitates straightforward evaluation of particle residence time distributions. There have been some studies that have compared the performance of MP-PIC compared to CFD-DEM. [Lu et al. \(2017\)](#) compared experiments with simulations using CFD-DEM and MP-PIC for a small-scale bubbling fluidized bed. The MP-PIC cases included the open-source MFiX code ([Garg and Dietiker, 2013](#)) and the commercial Barracuda (CPFD) software. They evaluated particle velocity profiles and found that only CFD-DEM reproduced the rising solids velocity distribution in line with the experiments. In contrast, MP-PIC in both MFiX and Barracuda predicted noticeably different particle velocities. Overall, they reported both quantitative and qualitative disagreement between MP-PIC and CFD-DEM for this small-scale system. Similar issues were also reported by [Liang et al. \(2014\)](#) where their CPFD MP-PIC model gave a reasonable solids velocity profile, but failed to capture bubble coalescence in bubbling fluidized beds. Based on these results, they recommended improvements to MP-PIC, especially to the particle stress model. In a lab-scale cold-flow spouted bed using two different air mass flow of 0.005 and 0.006 kg/s, [Stroh et al. \(2016\)](#) compared CFD-DEM with MP-PIC (Barracuda) against high-speed camera data, finding that while both methods captured the overall bed expansion and bubble development, CFD-DEM matched the flow-pattern details better (including gas channel formation and bubble collapse/bursting), whereas MP-PIC tended to over-predict particle velocities (especially at early times) and missed key structures such as the emerging gas channel and solids accumulation, with discrepancies becoming larger at the higher flow rate. Given to the poor performance of MP-PIC models, [Verma and Padding \(2020\)](#) introduced a new approach to MP-PIC called as Continuum particle model (CPM). This approach is similar to MP-PIC in treating both fluid and particle phases. The main difference with MP-PIC is that CPM (i) relies on a robust measurement of the local solids deformation rate, which is essential for accurate local stress estimation, and (ii) updates particle velocities using a simple formulation based on the local divergence of the solids stress tensor. They compared MP-PIC (Barracuda), CPM, and CFD-DEM for a pseudo-2D bubbling fluidized bed and found that CPM with the [Srivastava and Sundaresan \(2003\)](#) stress model reproduced CFD-DEM closely in time-averaged porosity patterns, bed height fluctuations, bubble size, and axial particle velocity profiles, whereas MP-PIC showed clear deviations, including smaller bubbles

and weak bubble coalescence, unrealistically dense packing, and incorrect particle velocity/flow structure compared with CFD-DEM.

In this work, we present a new implementation of the CPM, based on a face interpolation approach introduced in our previous work (Esgandari and Schneiderbauer, 2025), which represents a novel mapping strategy compared to the linear interpolation approach employed by Verma and Padding (2020) showing considerably improved predictions of bubbling and spout structures compared with MP-PIC. A further novelty of this work is the incorporation of a particle stress model based on the closure of Chialvo et al. (2012), including isotropic particle pressure as well as viscous and frictional particle stresses. This closure spans the quasi-static, intermediate, and collisional regimes while avoiding the evaluation of granular temperature required by the Srivastava and Sundaresan (2003) closure employed by Verma and Padding (2020). In addition, the Srivastava and Sundaresan (2003) closure does not consider the intermediate and collisional regimes, which would require the inclusion of granular temperature when using closures based on the kinetic theory of granular flows. The proposed CPM is systematically evaluated against MP-PIC (Barracuda), CFD-DEM, and experimental data for bubbling, single-spout, and triple-spout fluidized beds. In addition, a detailed comparison between CPM and CFD-DEM is performed in terms of time-averaged particle velocity, solids volume fraction, and particle mixing. Finally, the influence of the smoothing characteristic size δ_f on the predicted particle field data is investigated under different fluidization and spouting regimes.

2. Continuum particle model (CPM)

2.1. Fluid-phase equations

The volume-filtered governing equations for mass and momentum of the gas phase with considering particles presence are given by

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g) = 0, \quad (1)$$

$$\frac{\partial(\alpha_g \rho_g \mathbf{u}_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\alpha_g \nabla p_g + \nabla \cdot (\alpha_g \boldsymbol{\tau}_g) + \mathbf{F}^{drag} + \alpha_g \rho_g \mathbf{g}, \quad (2)$$

where ρ_g is the density of the fluid phase, $\mathbf{u}_g$ is the velocity of the fluid phase, p_g is the fluid phase pressure, $\mathbf{g}$ is the gravitational acceleration, and a Newtonian deviatoric stress is considered for the fluid phase stress-strain tensor, $\boldsymbol{\tau}_g$. Also, $\mathbf{F}^{drag}$ represents the interphase momentum exchange force which is the drag force. In this study, we implement $\mathbf{F}^{drag}$ in a semi-

implicit manner as explained in the supplementary material of our previous work (Esgandari and Schneiderbauer, 2025).

2.2. Particle-phase equations

The particle-phase momentum equation is

$$m_i \frac{d\mathbf{u}_{p,i}}{dt} = \mathbf{F}_i^{p-p} + \mathbf{F}_i^{g-p} + \mathbf{F}_i^{grav.}, \quad (3)$$

$$I_i \frac{d\boldsymbol{\omega}_{p,i}}{dt} = \mathbf{T}_i, \quad (4)$$

where m_i is the particle mass, $\mathbf{u}_{p,i}$ is the particle translational velocity, $\boldsymbol{\omega}_{p,i}$ is the particle rotational velocity, $\mathbf{T}_i$ is the torque. Moreover, $\mathbf{F}_i^{grav.}$ is the gravitational body force. The main distinction between CFD-DEM and CPM approaches lies on how particle-particle collision force, $\mathbf{F}_i^{p-p}$, is treated. In our CFD-DEM simulations, we evaluate the contact forces by adopting soft-sphere model. However, in CPM the particle-particle contact forces are evaluated from the divergence of the particle stress.

2.3. Particle-gas interaction force models

Particle-gas interaction forces, $\mathbf{F}_i^{g-p}$, are

$$\mathbf{F}_i^{g-p} = V_i \mathbf{F}_{drag,i} - V_i \nabla p_{g@i} - V_i \nabla \cdot \boldsymbol{\tau}_{g@i}, \quad (5)$$

where V_i is the particle volume. The first term on the right-hand side of Eq. (5), represents the fluid drag force applied to a particle, $\mathbf{F}_{drag,i} = \beta(\mathbf{u}_{g@i} - \mathbf{u}_{p,i})$, the second term denotes the pressure gradient force, and the third term shows the viscous force originating from the deviatoric fluid-phase stress tensor. In addition, @i denotes that the properties of the fluid phase are interpolated to the location of the particle i .

2.4. Particle stress model

The particle stresses arise from compressive, shearing, and elongation deformations of the particle system. The particle stress tensor, $\mathbf{S}_p$, composed from normal and shear terms, reads as

$$\mathbf{S}_p = p_p \mathbf{I} - 2\mu_p \text{dev } \mathbf{D}_p, \quad (6)$$

where $\mathbf{I}$ is the identity tensor, p_p is the normal stress (particle pressure), μ_p is the particle friction, and $\text{dev } \mathbf{D}_p = \mathbf{D}_p - \frac{1}{3} \text{tr}(\mathbf{D}_p) \mathbf{I}$. Here, an inertial-number-dependent friction coefficient

based on $\mu(I)$ -rheology could be used. However, because $\mu(I)$ -rheology is known to lack grid convergence and grid refinement may lead to numerical instabilities (Barker et al., 2015), we do not employ it here. The strain rate tensor is defined as, $\mathbf{D}_p = \frac{1}{2}(\nabla \mathbf{u}_p + (\nabla \mathbf{u}_p)^T)$. Verma and Padding (2020) adopted the stress model of Srivastava and Sundaresan (2003), while in the work, we use the particle stress model proposed by Chialvo et al. (2012). The Chialvo et al. (2012) includes isotropic particle pressure as well as viscous and frictional particle stresses. This closure spans the quasi-static, intermediate, and collisional regimes while avoiding the evaluation of granular temperature required by the Srivastava and Sundaresan (2003) closure for the frictional stress and by the kinetic theory model covering the collisional regime. This particle stress model is

$$p_p = \begin{cases} p_p^{\text{QS}} + p_p^{\text{int}} & \text{for } \alpha_p \geq \alpha_p^{\text{max}} \\ \left((p_p^{\text{inert}})^{-1} + (p_p^{\text{int}})^{-1} \right)^{-1} & \text{for } \alpha_p < \alpha_p^{\text{max}} \end{cases}, \quad (7)$$

where p_p^{QS} , p_p^{int} , and p_p^{inert} denote quasi-static, intermediate and inertial regimes contributions and take the form (Chialvo et al., 2012)

$$\frac{p_p^{\text{QS}} d_p}{k} = \alpha_{\text{QS}} \|\alpha_p - \alpha_p^{\text{max}}\|^{2/3} \quad (8)$$

$$\frac{p_p^{\text{int}} d_p}{k} = \alpha_{\text{int}} \hat{\gamma}_p^{1/2} \quad (9)$$

$$\frac{p_p^{\text{inert}} d_p}{k} = \frac{\alpha_{\text{inert}} \hat{\gamma}_p^2}{\|\alpha_p - \alpha_p^{\text{max}}\|^2} \quad (10)$$

where the scaled shear rate is defined as

$$\hat{\gamma}_p = \frac{2 \|\text{dev } \mathbf{D}_p\| d_p}{\sqrt{k/(\rho_p d_p)}}, \quad (11)$$

and d_p , k and α_p^{max} are the particle diameter, the particle stiffness, and the maximum packing. Furthermore, α_{QS} , α_{int} , and α_{inert} denote the model parameters. Following Schneiderbauer et al. (2015), substituting Eq. (11) into p_p^{inert} reveals that p_p^{inert} is not dependent on the particle stiffness which reads

$$p_p^{\text{inert}} = 4\rho_p \alpha_{\text{inert}} \left(\frac{\|\text{dev } \mathbf{D}_p\| d_p}{\alpha_p - \alpha_p^{\text{max}}} \right)^2. \quad (12)$$

2.5. Mapping and smoothing

To solve the fluid phase mass and momentum equations (Eqs. (1)-(2)), particle data including volume, velocity, and drag force should be volume-filtered (mapped) on the grid. The locally-averaged (mapped) quantity is obtained according to,

$$\alpha_p \tilde{\psi}(\mathbf{x}_q, t) = \sum_i^{N_p} \psi_i \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_q|) V_i \quad (13)$$

where $q = f$ represents the center of cell faces in case of GaussFace method which was introduced in our previous work (Esgandari and Schneiderbauer, 2025). Also, $\mathbf{x}_i$ is the position of the particle. Using $\psi_i = 1$, $\psi_i = \mathbf{u}_{p,i}$, and $\psi_i = \mathbf{F}_{drag,i}$ will lead to α_p , $\alpha_p \mathbf{u}_p$, and $\alpha_p \mathbf{F}^{drag}$. In GaussFace method, the particle data are distributed to the neighboring cells using weights evaluated based on a Gaussian kernel,

$$\mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{r^2}{2\sigma^2}} \quad (14)$$

where r is the distance between the particle center and the cell face centers (C_f) and the standard deviation of the kernel is defined as $\sigma = \Delta x / (2\sqrt{2\ln 2})$, such that the full width at half the height of the kernel is equal to grid size, Δx (Capecelatro and Desjardins, 2013). By normalizing the weights, the conservation of the particle data is ensured. In the next step, since in Finite Volume Method (FVM), the values in the cell centers, $\tilde{\psi}$, are required, the distributed data are summed with considering a face weight, ζ_f , to obtain the cell center value,

$$\alpha_p \tilde{\psi} = \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f \psi_i \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|) V_i \quad (15)$$

where N_f is the number of cell face and $\mathcal{F}_i$ represents the set of faces belonging to the cell containing the particle. The normalization is performed by applying $\mathcal{N}_i = \sum_{f \in \mathcal{F}_i} \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|)$. If the cell face is located in the outline of the domain (wall, inlet or outlet boundary) $\zeta_f = 1$, otherwise in internal faces, processor and periodic boundaries, $\zeta_f = 0.5$, leading to diffusion of the particle data from a cell to its neighbors. The grid-independency of CFD-DEM simulations using GaussFace mapping method and smoothing has been covered in our previous work (Esgandari and Schneiderbauer, 2025).

The following transient diffusion equation is solved to obtain smoother particle data fields after mapping is done,

$$\frac{\partial \tilde{\psi}}{\partial t} = \mathcal{D} \nabla^2 \tilde{\psi}, \quad (16)$$

where $\mathcal{D}$ is a diffusion coefficient and is evaluated using $\mathcal{D} = \delta_f^2 / (16 \ln 2 \Delta t)$ (Capecelatro and Desjardins, 2013). In this method, δ_f and Δt are the smoothing characteristic size and CFD time step, respectively. Furthermore, $\bar{\psi}$ indicates the smoothed field.

2.6. Numerical implementation of particle stress model

As can be deduced from Eq. (6), the shear (viscous) stress requires the evaluation of particle velocity gradient ($\nabla \tilde{\mathbf{u}}_{p,f}$) in the faces of computational cells. It can efficiently be calculated using the position and velocity of the individual particles using (Verma and Padding, 2020)

$$\nabla \tilde{\mathbf{u}}_{p,f} = \mathbf{G}_f^{-1} \cdot \mathbf{C}_f, \quad (17)$$

$$\mathbf{G}_f = \frac{1}{M_f} \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f m_{p,i} \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|) (\mathbf{r}_i - \mathbf{R}_{cm,f}) \otimes (\mathbf{r}_i - \mathbf{R}_{cm,f}), \quad (18)$$

$$\mathbf{C}_f = \frac{1}{M_f} \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f m_{p,i} \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|) (\mathbf{r}_i - \mathbf{R}_{cm,f}) \otimes (\mathbf{v}_i - \mathbf{V}_{cm,f}), \quad (19)$$

with

$$M_f = \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f m_{p,i} \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|), \quad (20)$$

$$\mathbf{R}_{cm,f} = \frac{1}{M_f} \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f m_{p,i} \mathbf{x}_i \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|), \quad (21)$$

$$\mathbf{V}_{cm,f} = \frac{1}{M_f} \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f m_{p,i} \mathbf{u}_{p,i} \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|), \quad (22)$$

where m_p , $\mathbf{G}$, and $\mathbf{C}$ are the gyration tensor and position-velocity correlation tensor of all N_p particles present in the computational cell. Also, M , $\mathbf{R}_{cm}$, and $\mathbf{V}_{cm}$ denote the total particle mass, and center of mass of position and velocity of all particles present inside a computational cell. It needs to be mentioned that all quantities as marked by the subscript f are evaluated at the center of the faces of the grids, this is due to the fact that our mapping method evaluates the variables on the faces.

The particle-particle contact force in CPM, $\mathbf{F}_i^{p-p}$, can be calculated with

$$\mathbf{F}_i^{p-p} = - \left(\frac{m_i}{\alpha_{p@i} \rho_p} \nabla \cdot \mathbf{S}_p \right)_{@i}, \quad (23)$$

where m_i is the particle mass. According to Eq. (6), the particle stress tensor is comprised

from normal and shear stresses, therefore $\mathbf{F}_i^{p-p}$ can be divided into two parts

$$\mathbf{F}_i^{p-p} = \mathbf{F}_i^{\nabla p_p} + \mathbf{F}_i^{\nabla \cdot (\text{dev } \mathbf{D}_p)} = - \left(\frac{m_i}{\alpha_{p@i} \rho_p} \nabla p_p \right)_{@i} + \left(\frac{2\mu_p m_i}{\alpha_{p@i} \rho_p} \nabla \cdot (\text{dev } \mathbf{D}_p) \right)_{@i}. \quad (24)$$

It need to be mentioned that ∇p_p and $\nabla \cdot (\text{dev } \mathbf{D}_p)$ are evaluated directly from the face values which is obtained from the adopted GaussFace mapping method and are interpolated to the location of the particle. Therefore, the particle velocity update due to the normal stress can be evaluated using

$$\mathbf{u}_{p,i}^{\nabla p_p} = \frac{-\Delta t \nabla p_{p@i}}{\rho_p \alpha_{p@i}}, \quad (25)$$

where Δt is the time step. The particle velocity change due to the normal stress is evaluated only when the relative particle velocity, $\mathbf{u}_{rel,p} = \mathbf{u}_{p,i} - \tilde{\mathbf{u}}_{p@i}$, is directed toward increasing volume fraction (i.e., $\mathbf{u}_{rel,p} \cdot \nabla \alpha_{p@i} > 0$); otherwise, $\mathbf{u}_{p,i}^{\nabla p_p}$ is set to zero. In the second step, the velocity update obtained from Eq. (25) may become large due to high values of $\nabla p_{p@i}$. Therefore, the particle velocity must be bounded, which can be mathematically expressed as (Verma and Padding, 2020)

$$\mathbf{u}_{p,i}^{\nabla p_p} = \text{MinMod} \left[\mathbf{u}_{p,i}^{\nabla p_p}, -(1 + e_p)(\mathbf{u}_{rel,p}) \frac{|\mathbf{u}_{p,i}|}{|\mathbf{u}_{rel,p}|} \right]. \quad (26)$$

The MinMod operator returns zero if its inputs have opposite signs, otherwise it returns the minimum of the arguments. Note that the particle velocity magnitude is computed while accounting for the particle coefficient of restitution, e_p , which defines particle-particle collision characteristics. In this way, the continuum particle normal stress gradient applied to a discrete particle is limited by the particle velocity relative to the mean flow velocity, and it becomes dominant close to dense particle packing. Based on the calculated $\mathbf{u}_{p,i}^{\nabla p_p}$, we can obtain

$$\mathbf{F}_i^{\nabla p_p} = \frac{\mathbf{u}_{p,i}^{\nabla p_p} m_i}{\Delta t} \quad (27)$$

The second part of the particle velocity update stems from the shear stress which is calculated from

$$\mathbf{u}_{p,i}^{\nabla \cdot (\text{dev } \mathbf{D}_p)} = \frac{\nabla \cdot (\text{dev } \mathbf{D}_p \cdot \mathbf{S}_f) \Delta t}{\rho_p \alpha_{p@i}}. \quad (28)$$

Then, $\mathbf{F}_i^{\nabla \cdot (\text{dev } \mathbf{D}_p)}$ can be computed from

$$\mathbf{F}_i^{\nabla \cdot (\text{dev } \mathbf{D}_p)} = \frac{\mathbf{u}_{p,i}^{\nabla \cdot (\text{dev } \mathbf{D}_p)} m_i}{\Delta t}. \quad (29)$$

2.7. Particle-wall contacts

Particles are allowed to collide with the wall so that they remain inside the computational domain. Because the chosen time step is relatively large in CPM simulations, particle-wall interactions can be modeled using a hard-sphere collision approach. As an example, consider a particle with velocity, v_i . Before it collides with a wall, its velocity can be decomposed into tangential and normal components relative to the wall, denoted by $v_{i,t}$ and $v_{i,n}$, respectively. The hard-sphere model is defined by three collision parameters: the normal restitution coefficient e_n , the tangential restitution coefficient β_0 , and the friction coefficient μ . Using these parameters, the post-collision particle velocity is computed from Eqs. (30) and (31).

$$v'_{i,n} = -e_n v_{i,n} \quad (30)$$

$$v'_{i,t} - v_{i,t} = \begin{cases} -\frac{2}{7}(1 + \beta_0)v_{i,t}, & \text{if } -\mu(1 + e_n)v_{i,n} \geq \frac{2}{7}(1 + \beta_0)v_{i,t}, \\ \mu(1 + e_n)v_{i,n}, & \text{otherwise.} \end{cases} \quad (31)$$

2.8. Interphase drag force

Interphase drag force is the important source of momentum exchange between the phases. Table 1 summarizes two different interphase drag coefficients studied in this paper. The interphase drag coefficient correlations are either obtained through measurements of pressure drop and terminal velocity of sedimenting particles or via accurate direct numerical simulations (DNS). The model of Wen and Yu (1966) is one of the empirically obtained interphase drag models which is widely used in simulations of fluid-solid systems. The other drag correlation, Beetstra et al. (2007) in the Table 1 was obtained from DNS. It is clear that all interphase drag models are functions of Re number and α_p . Furthermore, it should be mentioned that none of the interphase drag correlations listed in Table 1 includes the pressure gradient force effect.

Table 1: Interphase drag coefficient correlations

Correlation	Interphase drag coefficient	Re	α_p
Wen and Yu (1966)	$\beta = \frac{3}{4}C_D \frac{\rho_f \alpha_f \alpha_p \mathbf{u}_f - \mathbf{u}_p }{d_p} \alpha_f^{-2.65}$ $\text{with } C_D = \begin{cases} 24/Re (1 + 0.15Re^{0.687}) & Re < 1000 \\ 0.44 & Re \geq 1000 \end{cases}$ $Re = \frac{\alpha_f \rho_f d_p \mathbf{u}_f - \mathbf{u}_p }{\mu_f}$		
Beetstra et al. (2007)	$\beta = 180 \frac{\mu_f \alpha_p^2}{d_p^2 \alpha_f} + 18 \frac{\mu_f \alpha_f^3 \alpha_p (1 + 1.5\sqrt{\alpha_p})}{d_p^2}$ $+ 0.31 \frac{\mu_f \alpha_p Re [\alpha_f^{-1} + 3\alpha_f \alpha_p + 8.4Re^{-0.343}]}{d_p^2 \alpha_f [1 + 10^3 \alpha_p Re^{-0.5-2\alpha_p}]}$	$20 < Re < 1000$	up to 0.6

3. Mixing indices

Evaluating mixing in a system is essential because it provides a quantitative measure of how uniformly particle species are distributed, which directly affects process performance and final product quality. In granular systems, reliable mixing assessment also helps identify segregation mechanisms and supports the optimisation of industrial operations such as those in pharmaceutical, agricultural, and chemical applications. In this paper, we will evaluate the degree of mixing in our simulations, using Lacey index and neighbour distance method.

The Lacey index (Lacey, 1954), denoted by M_{LI} , is a widely used grid-based mixing index for quantifying the degree of mixing in binary particulate systems. In this approach, the computational or experimental domain is divided into S non-empty samples or grid cells, and the local composition in each sample is compared with the global composition of the system. Let $P = P_a + P_b$ denote the total number of particles in the system, while P_a and P_b represent the numbers of particles of type a and type b, respectively. For the i -th sample, $P_i = P_{a,i} + P_{b,i}$ denotes the total number of particles, and $P_{a,i}$ and $P_{b,i}$ denote the numbers of particles of type a and type b within that sample. The global fraction of type a particles is represented by $f_a = P_a/P$, while the corresponding local fraction in sample i is $f_{a,i} = P_{a,i}/P_i$. The Lacey index is based on the variance of these local particle fractions across all samples. The variance of local particle fractions is calculated as

$$\sigma^2 = \frac{1}{S-1} \sum_{i=1}^S (f_{a,i} - f_a)^2. \quad (32)$$

This variance is large when the system is segregated, since the local fractions differ strongly from one sample to another, and small when the system is well mixed, since the local fractions approach the global mean. To normalize the result, Lacey (1954) introduced two reference variances: the variance of a theoretically fully mixed system,

$$\sigma_m^2 = \frac{f_a(1-f_a)}{n} \quad (33)$$

where n is the average number of particles per sample, and the variance of a fully segregated system,

$$\sigma_s^2 = f_a(1-f_a). \quad (34)$$

Using these reference values, the Lacey index is defined as,

$$M_{\text{LI}} = \frac{\sigma^2 - \sigma_s^2}{\sigma_m^2 - \sigma_s^2}. \quad (35)$$

In this normalized form, $M_{\text{LI}} = 0$ corresponds to a completely segregated state, whereas $M_{\text{LI}} = 1$ corresponds to a fully mixed state. This index performs best when the solid fraction is fairly uniform and when each sample contains a sufficient number of particles to ensure statistically reliable results (Füvesi et al., 2025).

The Neighbour Distance Method (NDM) belongs to the class of distance-based mixing indices, which evaluate mixing by using the spatial positions of particles directly (Füvesi et al., 2025). In numerical simulations, particle positions are readily available, making these methods attractive because they do not require additional procedures such as binning. Instead, they quantify mixing through distances between particles or between particles and reference positions. Among these methods, the NDM assesses the extent of mixing by monitoring how initially neighbouring particles separate over time. At the initial state, each particle is assigned its closest neighbour, forming one set of particle pairs, while a second set is formed by randomly pairing particles throughout the system. The distances between the neighbouring pairs are denoted by $r_{n,j}$, whereas the distances between the random pairs are denoted by $r_{r,j}$. The first set reflects the local spreading of particles caused by mixing, while the second set provides a normalization that accounts for possible changes in the overall system size. In this way, the NDM provides a normalized measure of particle dispersion, with values ranging from 0 for a segregated state to 1 for a mixed state. An important advantage of this method is that it can evaluate mixing for the entire system without requiring the prior selection of a specific particle type to trace, which makes it applicable to a broader range of system compositions (Füvesi et al., 2025). A key limitation of NDM is that, because it relies only on geometric distances between particle pairs, it does not directly account for particle-type differences. As a result, it may not capture segregation driven by properties such as particle size or density. The NDM index is defined as

$$M_{\text{NDM}} = \frac{\sum_{j=1}^P (r_{n,j} - d_{n,j})}{\sum_{j=1}^P (r_{r,j} - d_{r,j})} \quad (36)$$

where P is the total number of particles, $r_{n,j}$ is the distance between particle j and its initially closest neighbour, $r_{r,j}$ is the distance between particle j and its randomly assigned pair, and $d_{n,j}$ and $d_{r,j}$ are the average particle diameters of the corresponding pairs.

4. Results and discussion

In this section, all CPM simulations were performed using first-order implicit Euler time discretization. In addition, the simulations presented in this paper employed second-order spatial schemes for both the diffusion (Gauss linear (Greenshields and Weller, 2022)) and advection (linearUpwindV (Greenshields and Weller, 2022)) terms in the Navier–Stokes equations.

For pressure-velocity coupling, the PIMPLE algorithm, which combines the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) and the Pressure Implicit with Splitting of Operators (PISO) methods, was used. In the CPM framework, the fluid-phase equations are solved on an Eulerian grid in OpenFOAM, while the particles are tracked individually in a Lagrangian framework using LIGGGHTS. The coupling between the fluid and particle phases is handled through CFDEMcoupling. In this work, we treat the interphase momentum exchange term in Eq. (2), $\mathbf{F}^{drag}$, in a semi-implicit manner which reads as

$$\mathbf{F}^{drag^{n+1}} = \underbrace{\tilde{\mathbf{F}}_{drag}^n + \tilde{\beta} \mathbf{u}_g^n}_{\text{Explicit part}} - \underbrace{\tilde{\beta} \mathbf{u}_g^{n+1}}_{\text{implicit part}}, \quad (37)$$

where

$$\begin{aligned} \tilde{\mathbf{F}}_{drag}^n &= \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f \beta_i (\mathbf{u}_{p,i}^n - \mathbf{u}_{g@i}^n) \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|), \\ \tilde{\beta} &= \sum_i^{N_p} \frac{1}{\mathcal{N}_i} \sum_{f \in \mathcal{F}_i}^{N_f} \zeta_f \beta_i \mathcal{G}(|\mathbf{x}_i - \mathbf{x}_f|), \end{aligned} \quad (38)$$

where the superscripts " n " and " $n + 1$ " represent the explicit (old time) and implicit (new time) quantities. As can be seen from Eq. (37), in order to handle $\mathbf{F}^{drag}$ in a semi-implicit manner, an explicit term involving $\mathbf{u}_g$ is incorporated first, followed by the subtraction of its implicit form. Moreover, the particle velocity, $\mathbf{u}_{p,i}$, used in evaluating the drag force is treated explicitly.

4.1. Bubbling fluidized bed of Gopalan et al. (2016)

4.1.1. Simulation settings

The experimental data from bubbling fluidized bed of Gopalan et al. (2016) are adopted to validate the performance of CPM. The simulation parameters and material properties are listed in Table 2. The geometry of the fluidized bed can be seen in Fig. 1. A grid size of $\sim 4.6d_p$, corresponding to $16 \times 5 \times 66$ cells in x -, y -, and z -direction, is used. This grid spacing size was chosen based on the grid size sensitivity studies of Verma and Padding (2020), Ayeni et al. (2016), and Lu et al. (2017). The total number of Geldart D particles were 95000. The

simulations were performed for a duration of 20 s to ensure that a statistical steady state is attained. The statistics were averaged over time from 5 s to 20 s. No-slip boundary condition was applied to the gas phase velocity at the walls. At the inlet of the bed, uniform gas velocity was specified and atmospheric pressure was used at the top of outlet. The computational time for 1 s of simulation on 16-core CPU with 2.6 GHz frequency in case of CPM and CFD-DEM simulations was 420 s and 3340 s, respectively.

Table 2: Simulation parameters related to bubbling fluidized bed of [Gopalan et al. \(2016\)](#).

Property	Value	Unit
d_p	3.256	mm
μ_f	1.8×10^{-5}	$\text{kg m}^{-1} \text{s}^{-1}$
ρ_f	1.2	kg m^{-3}
ρ_p	1131	kg m^{-3}
g	9.81	m s^{-2}
e_{p-p}	0.8	-
μ_{p-p}	0.3	-
α_{QS}	0.1	-
α_p^{max}	0.65	-
α_{int}	0.1	-
α_{inert}	0.04	-
k	1000	N m^{-1}
Δt	0.001	s

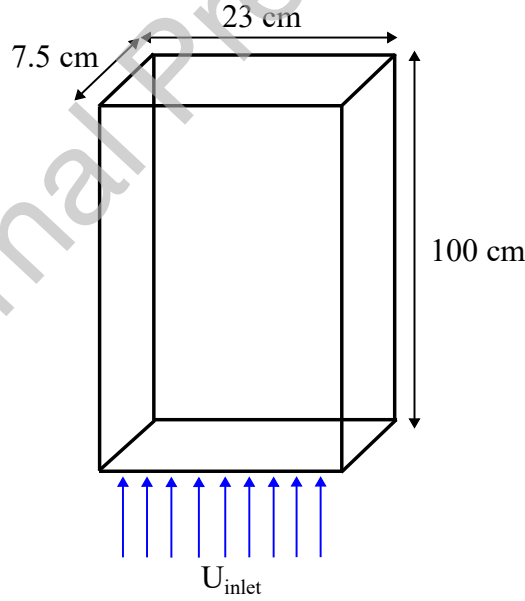


Fig. 1: The geometry of bubbling fluidized bed of [Gopalan et al. \(2016\)](#). The U_{inlet} is 3.28 m s^{-1} .

4.1.2. Validation results

In order to examine the effect of interphase drag models on hydrodynamics of the fluidized bed, the simulations with the interphase drag correlations of Table 1 are performed. Fig. 2 compares the time-averaged vertical particle velocity extracted from CPM and MP-PIC (Bar-racuda) simulations with the experimental measurements of [Gopalan et al. \(2016\)](#). All CPM

simulations, using either drag model, successfully capture the correct bubbling flow regime of the bed. In these simulations, the bubbles rise mainly through the center of the bed, while their motion causes particles near the side walls to move downward. For the CPM ($\delta_f = 7d_p$), MP-PIC, CPM with GaussFace mapping ($\delta_f = 7d_p$, [Harris and Crighton \(1994\)](#)), and CPM with PIC mapping ($\delta_f = 7d_p$, [Harris and Crighton \(1994\)](#)), the RMSE values relative to the experimental data are 0.069, 0.244, 0.343, and 0.245, respectively, when using the [Wen and Yu \(1966\)](#) drag model, and 0.274, 0.259, 0.493, and 0.233, respectively, when using the [Beetstra et al. \(2007\)](#) drag model. Quantitatively, CPM simulation using [Wen and Yu \(1966\)](#) drag model and $\delta_f = 7d_p$ with [Chialvo et al. \(2012\)](#) stress model matches relatively well with experiments than the simulation with [Beetstra et al. \(2007\)](#) drag model. The particle velocity is over-predicted when using the drag model of [Beetstra et al. \(2007\)](#) because, for particle volume fractions below $\alpha_p = 0.4$, this model gives higher drag coefficients than [Wen and Yu \(1966\)](#) model as reported by [Liu and van Wachem \(2019\)](#). As can be seen, MP-PIC simulations using Barracuda cannot capture the correct bed dynamics. Fig. 3 shows that the MP-PIC simulation in Barracuda produces small bubbles, whereas the CPM using [Chialvo et al. \(2012\)](#) stress model predicts larger bubbles. The reason lies in the particle stress model incorporated in the Barracuda, which is from the work of [Harris and Crighton \(1994\)](#) and defined as

$$\mathbf{S}_p = \frac{P^* \alpha_p^\beta}{\max(\alpha_{\max} - \alpha_p, \delta)} \mathbf{I}. \quad (39)$$

We adopted $P^* = 1$, $\beta = 2$, and $\delta = 10^{-8}$ in our MP-PIC simulations. However, modifying the values of P^* and β did not improve the results as presented in [Appendix A](#). It can be seen from Eq. (39) that the model includes only isotropic particle pressure and neglects viscous/frictional particle stresses, so it misses important resistance against shearing and the elongational deformation in dense regions. [Lu et al. \(2017\)](#) obtained a particle velocity profile similar to that predicted by MP-PIC using the MFiX software. We further investigated the effect of this simplified stress model in the CPM. We perform CPM simulations with a particle-in-cell (PIC) mapping strategy, whereby the particle data is attributed to the cell in which the particle centroid resides. To ensure consistency with the MP-PIC framework, the particle-phase stress is modeled using the formulation of [Harris and Crighton \(1994\)](#). As shown in Fig. 2, the results are comparable to those obtained with MP-PIC. Moreover, the instantaneous particle distribution predicted by CPM using the [Harris and Crighton \(1994\)](#) stress model together with the PIC mapping method closely resembles the MP-PIC result, as illustrated in Fig. 3. In addition, we change the mapping method from PIC to GaussFace using [Harris and Crighton](#)

(1994) stress model. Our results indicate that Harris and Crighton (1994) stress model using GaussFace mapping method over-predicts the upward particle velocity in the bed and produces large bubble sizes as is evident in Fig. 3. These observations suggest that to improve the MP-PIC performance, one needs to use an appropriate particle data mapping and particle stress closure together. Therefore, in the remainder of this paper, the Harris and Crighton (1994) stress model and PIC mapping are not employed in the CPM simulations.

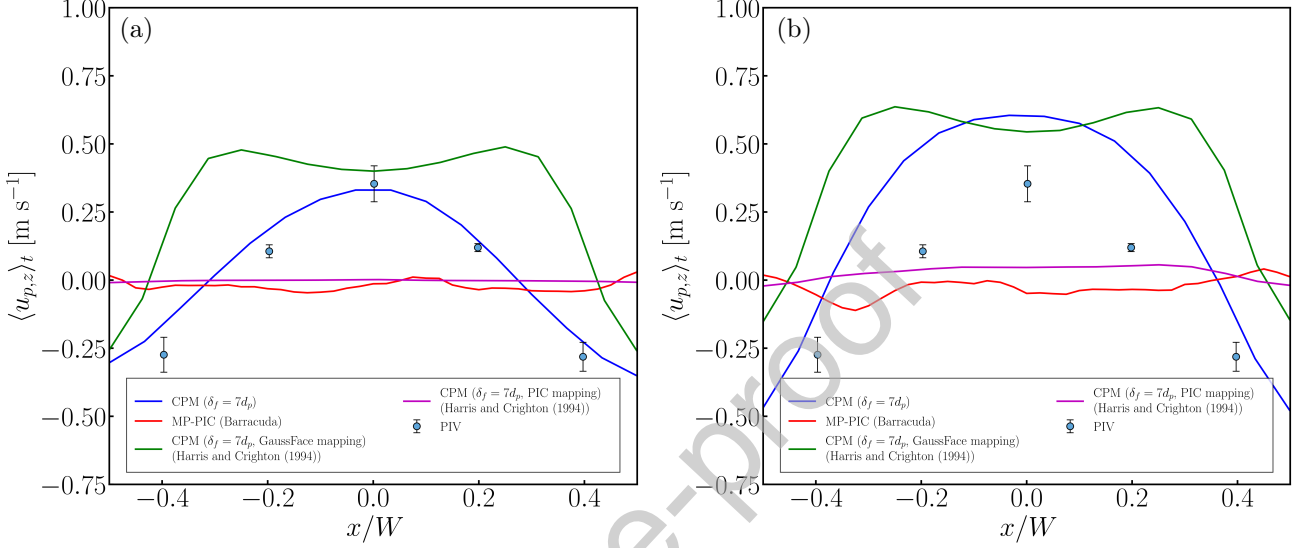


Fig. 2: Comparison of the time-averaged vertical particle velocity obtained from CPM using Chialvo et al. (2012) stress model, CPM using Harris and Crighton (1994) stress model and GaussFace mapping method, CPM using Harris and Crighton (1994) stress model and PIC mapping method, and MP-PIC (Barracuda) with the experimental data of Gopalan et al. (2016) at $z = 0.0762$ m. (a) simulations using Wen and Yu (1966) drag model and (b) simulations using Beetstra et al. (2007) drag model.

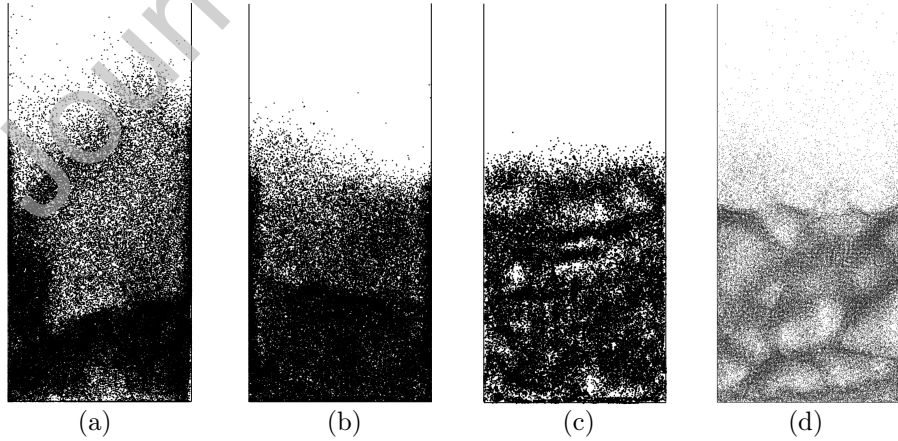


Fig. 3: Instantaneous particle distribution at $t = 10$ s from (a) CPM using Chialvo et al. (2012) stress closure, (b) CPM using Harris and Crighton (1994) stress closure and GaussFace mapping method, (c) CPM using Harris and Crighton (1994) stress closure and PIC mapping method, and (d) MP-PIC (Barracuda) in Gopalan et al. (2016) fluidized bed.

4.1.3. Effect of different smoothing characteristic sizes (δ_f) on CPM simulations

To ensure numerical stability, smoothing of the particle data fields is essential (Pirker et al., 2011; Esgandari et al., 2024). In the validation section, the CPM simulations were performed using a filter size of $\delta_f = 7d_p$. However, it is important to examine how the results change when different filter sizes are used. To investigate this, additional simulations were carried out without smoothing and with $\delta_f = 5d_p$, $7d_p$, and $10d_p$. Furthermore, based on the CPM validation results, we conducted a CFD-DEM simulation using Wen and Yu (1966) drag model with $\delta_f = 7d_p$ in order to compare the CPM approach against a higher-fidelity simulation method. This simulation-experiment synergy in understanding complex flow mechanisms has been used in previous literature (Su et al., 2026). To be consistent with the CPM simulations, particle rotation was not considered in the CFD-DEM simulations. The effect of particle rotation on the predictions of CFD-DEM simulations is presented in Appendix B. The details of the CFD-DEM methodology are available in our previous studies (Esgandari et al., 2025; Esgandari and Schneiderbauer, 2025).

Time-averaged particle velocity and volume fraction profiles

Fig. 4(a) shows the time-averaged particle velocity profiles. The RMSE values for CFD-DEM, CPM without smoothing, and CPM with $\delta_f = 5d_p$, $7d_p$, and $10d_p$ are 0.032, 0.112, 0.104, 0.069, and 0.158, respectively. Without smoothing, the predicted particle velocity does not agree well with the experimental and CFD-DEM data. As the δ_f increases up to $7d_p$, the agreement improves, particularly near the side walls. However, when δ_f is further increased to $10d_p$, the velocity profile changes from symmetric to asymmetric. This suggests that the bubbles predominantly move toward the left side of the bed, which is inconsistent with the experimental and CFD-DEM observations. Overall, the simulations are able to capture the bubbling flow regime in the fluidized bed independent of the smoothing characteristic length. However, best agreement of the particle velocity profile with the experimental data is achieved using $\delta_f = 7d_p$. Fig. 4(b) presents the laterally and time-averaged particle volume fraction along the bed height. The lateral average is obtained by averaging over all cells in the bed cross-section at each vertical position. Overall, the solids volume fraction is highest near the bottom of the bed and decreases gradually with height. It is also observed that the bed height predicted by CFD-DEM is slightly larger than that predicted by the CPM simulations. Although the CPM result with $\delta_f = 10d_p$ appears to match the CFD-DEM profile, this agreement is disregarded because the same case does not reproduce the bed dynamics correctly, particularly the vertical particle velocity. Increasing δ_f up to $7d_p$ leads to bubble eruption at higher elevations, causing

the predicted solids volume fraction profile to more closely match the CFD-DEM result.

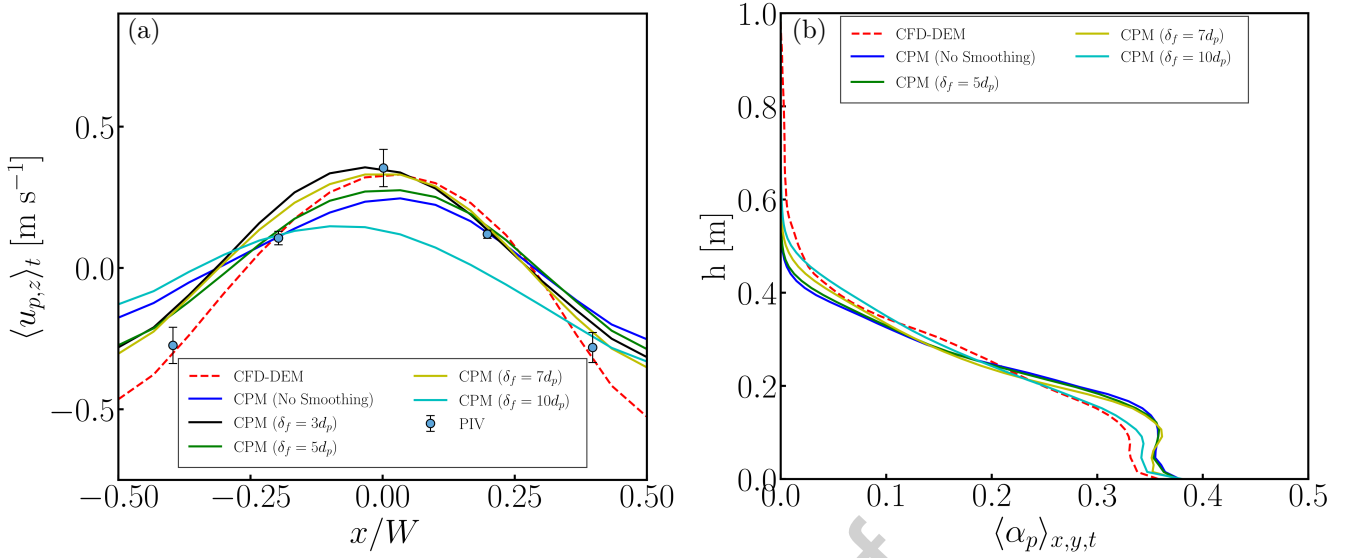


Fig. 4: Comparison of the (a) time-averaged vertical particle velocity obtained from CFD-DEM and CPM with the experimental data of Gopalan et al. (2016) at $z = 0.0762$ m and (b) laterally and time-averaged particle volume fraction along the bed height from CFD-DEM and CPM simulations with different δ_f values.

Particle mixing

Fig. 5 shows the mixing behavior obtained from CFD-DEM and CPM simulations at different δ_f values, evaluated using both the Lacey index and the nearest distance method (NDM). Based on the cell size sensitivity study presented in Appendix C, a grid of $(16 \times 5 \times 80)$ cells was selected for calculating the Lacey index. This configuration resulted in an average of approximately 20 particles per non-empty cell. Initially, the bed particles were divided into two types with equal numbers of particles and arranged along the bed height, so the system started from a segregated state.

As the simulation progresses, the particles gradually move from this segregated state toward a mixed state, which is also visible in Fig. 6. However, the two mixing indices do not show exactly the same trend. The Lacey index does not reach the value corresponding to a fully mixed state, while the NDM does. In addition, the Lacey index predictions show relatively large fluctuations near the maximum mixing degree. This suggests that the Lacey index is not well suited for assessing mixing in fluidized beds, where dense and dilute regions coexist. In particular, the dilute regions create grid cells with very low particle concentration, which can distort the cell-based statistics and lead to artificial behavior in the Lacey index (Füvesi et al., 2025).

Looking at the NDM results, the CPM simulations show only small differences in mixing behavior across the different δ_f values. The results also indicate that mixing develops more

slowly in the CFD-DEM simulations than in the CPM simulations. For example, in Fig. 6 at $t = 2.5$ s, CFD-DEM still shows a noticeable unmixed cluster of yellow particles as marked by the red circle, whereas the CPM simulation already appears fully mixed at the same time. This slower mixing in CFD-DEM is likely related to the way particle contacts are modeled. In CFD-DEM, particle interactions are described using a nonlinear Hertzian contact model, which leads to higher energy dissipation during collisions. By contrast, CPM represents particle contacts through a particle stress closure. Because this approach does not resolve individual particle contacts, it cannot capture contact force chains that develop in densely packed regions. Examining the granular temperature profiles within the bed can help explain why CPM predicts faster mixing than CFD-DEM, as shown in Fig. 7. The granular temperature was calculated using the method explained in our previous studies (Esgandari and Schneiderbauer, 2025; Esgandari et al., 2025). It can be seen that both CFD-DEM and CPM predict a similar granular temperature trend, with the highest values occurring at the center of the bed. However, CFD-DEM predicts considerably lower granular temperature values. This difference stems from the explicit resolution of inelastic particle-particle collisions in CFD-DEM, which are one of the main sources of granular temperature dissipation, as discussed in our previous work (Esgandari et al., 2025).

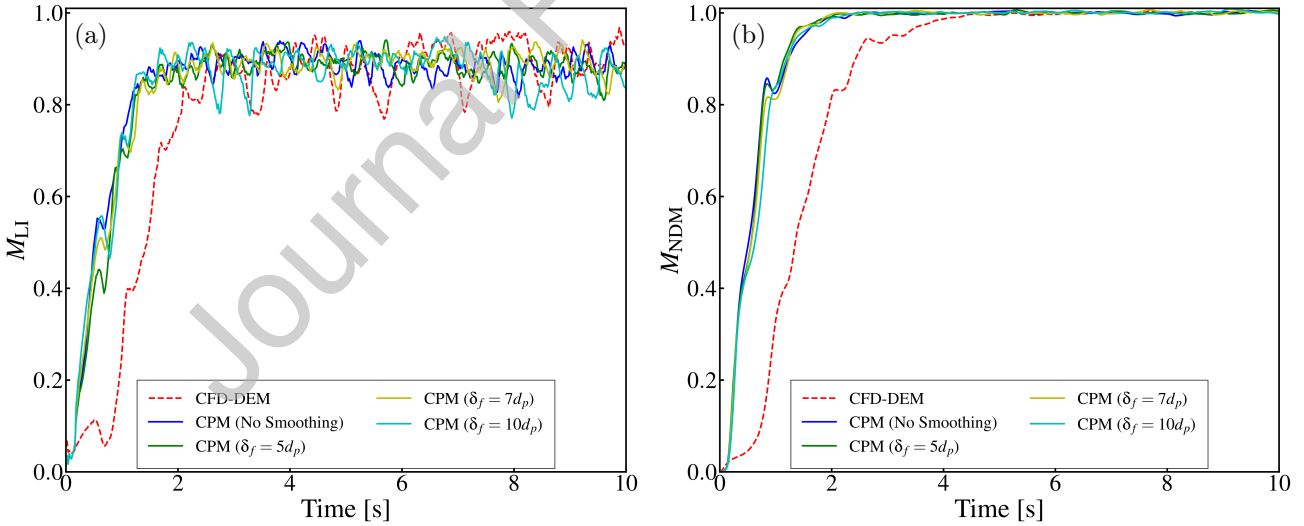


Fig. 5: Comparison of the mixing degree obtained from (a) Lacey index and (b) Nearest distance method from CFD-DEM and CPM simulations with different δ_f values in the fluidized bed.

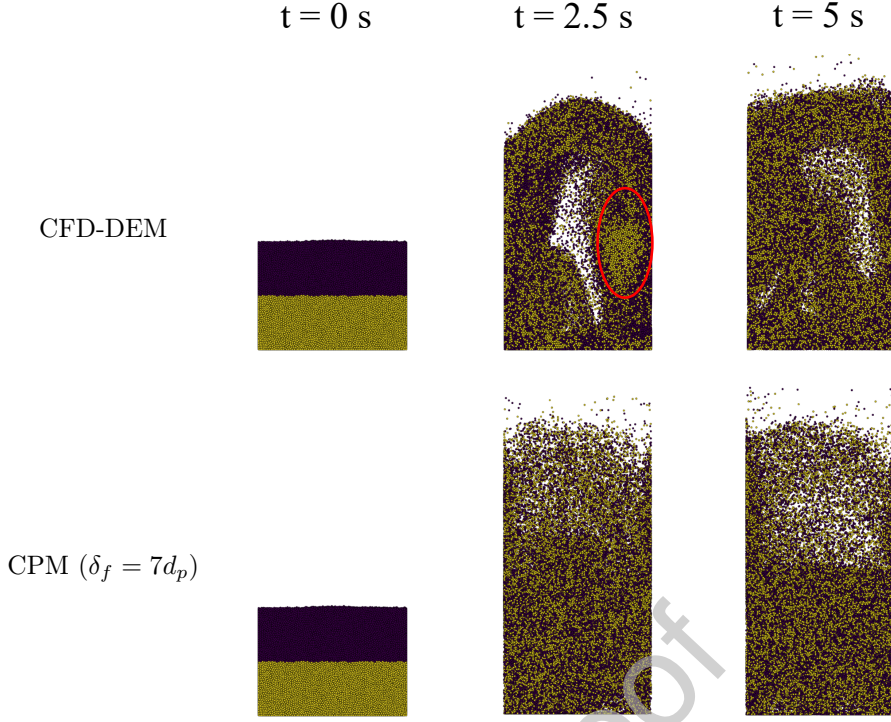


Fig. 6: Comparison of the mixing of the particles obtained from CFD-DEM and CPM ($\delta_f = 7d_p$) at different simulation instants in the fluidized bed.

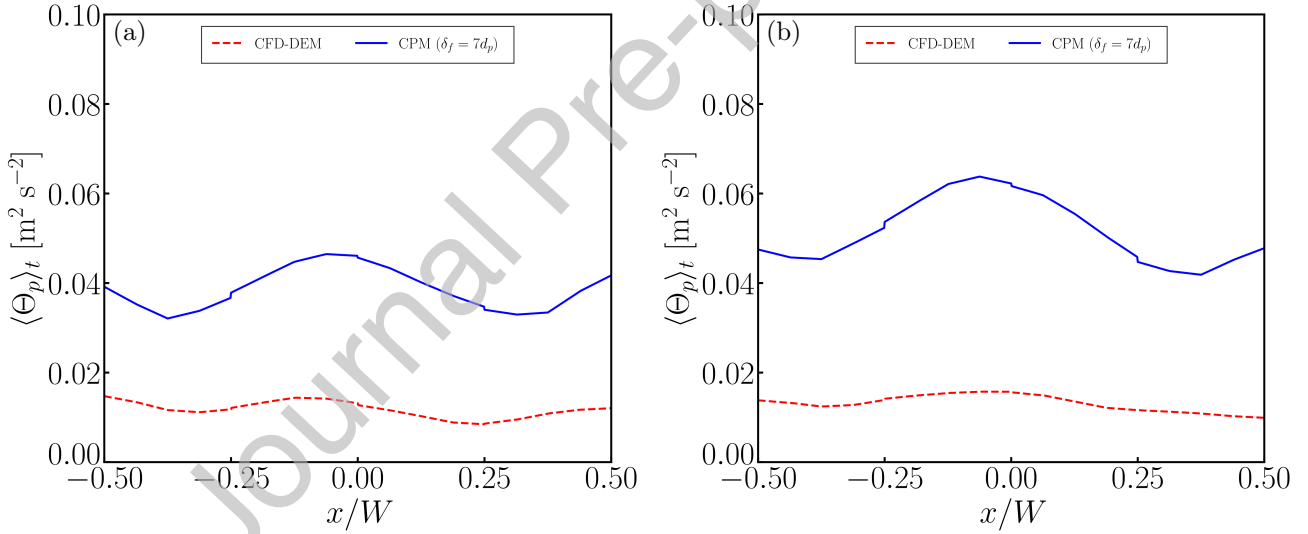


Fig. 7: Comparison of the time-averaged granular temperature obtained from CFD-DEM and CPM ($\delta_f = 7d_p$) at (a) $z = 0.05$ m and (b) $z = 0.1$ m in the fluidized bed.

4.2. Single-spout fluidized bed of Link et al. (2008)

4.2.1. Simulation settings

We choose to investigate the performance of the CPM and MP-PIC (Barracuda) simulations against experiments in a single-spout fluidized bed. To this end, we adopt the particle velocity data obtained using Positron Emission Particle Tracking (PEPT) method in the single-spout fluidized bed experiments of Link et al. (2008). The geometry of the bed is presented in Fig. 8. The spouting gas and background gas velocities corresponding to Jet-in-fluidized bed flow

regime are 65 m s^{-1} and 3.5 m s^{-1} . According to Link et al. (2008) observations, in jet-in-fluidized-bed regime, a spout channel forms within the bed while small bubbles emerge in the annulus, interacting with one another and ultimately leading to the formation of a fountain and the spout channel closes halfway up (Link et al., 2008). For all simulations a grid resolution of $21 \times 14 \times 100$ leading to $1.82d_p \times 1.5d_p \times 2.5d_p$ grid size was employed. This grid size is based on the grid sensitivity study of Yang et al. (2014) and which was adopted in previous works (Link et al., 2008; Hoorijani et al., 2024) as well. The material properties and simulation parameters are listed in Table 3. The total number of Geldart D particles in the bed is 44800. The simulations were ran for 15 s to achieve a statistically steady state, and the statistics were averaged from 5 s to 15 s. No-slip boundary condition was employed on the gas phase at the walls. At the spout and background inlets, a uniform gas velocity was specified, whereas atmospheric pressure was applied at the top outlet. The computational time for 1 s of simulation on 16-core CPU with 2.6 GHz frequency in case of CPM and CFD-DEM simulations was 442 s and 1225 s, respectively.

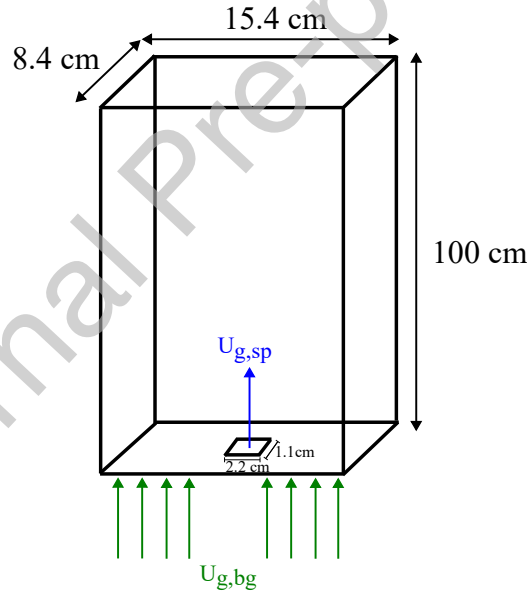


Fig. 8: The geometry of single-spout fluidized bed of Link et al. (2008). The $U_{g,sp}$ is 65 m s^{-1} and $U_{g,bg}$ is 3.5 m s^{-1} .

4.2.2. Validation results

Fig. 9 compares the time-averaged particle velocity predicted by MP-PIC (Barracuda) and CPM without smoothing, using the Wen and Yu (1966) drag model and the Beetstra et al. (2007) drag model, against the PEPT measurements of Link et al. (2008). Qualitatively, all simulations capture the key features of the spouting flow regime. In the spout region, particles are carried upward by the gas flow, then fall back onto the bed surface in the fountain region

Table 3: Simulation parameters related to single-spout fluidized bed of [Link et al. \(2008\)](#).

Property	Value	Unit
d_p	4.04	mm
μ_f	1.8×10^{-5}	$\text{kg m}^{-1} \text{s}^{-1}$
ρ_f	1.2	kg m^{-3}
ρ_p	2596	kg m^{-3}
g	9.81	m s^{-2}
e_{p-p}	0.8	-
μ_{p-p}	0.3	-
α_{QS}	0.1	-
α_p^{max}	0.65	-
α_{int}	0.1	-
α_{inert}	0.04	-
k	1000	N m^{-1}
Δt	0.00025	s

497 due to gravity. They then move downward through the annulus and re-enter the spout near
 498 the gas inlet. At $z = 0.15$ m, the RMSE values relative to the experimental data for CPM
 499 without smoothing and MP-PIC are 0.243 and 0.253, respectively, with the [Wen and Yu \(1966\)](#)
 500 drag model, and 0.185 and 0.221, respectively, with the [Beetstra et al. \(2007\)](#) drag model.
 501 At $z = 0.15$ m, the CPM results without smoothing show that the [Beetstra et al. \(2007\)](#) drag
 502 model predicts higher particle velocities in the spout region than the [Wen and Yu \(1966\)](#) model,
 503 leading to better agreement with the experimental data. The MP-PIC (Barracuda) simulations
 504 also agree well with the experiments in the spout region; however, in the annulus region, they
 505 significantly under-predict the downward particle velocity compared to both the experiments
 506 and the CPM results. At $z = 0.25$ m, the RMSE values relative to the experimental data
 507 for CPM without smoothing and MP-PIC are 0.326 and 0.594, respectively, with the [Wen](#)
 508 [and Yu \(1966\)](#) drag model, and 0.231 and 0.547, respectively, with the [Beetstra et al. \(2007\)](#)
 509 drag model. At $z = 0.25$ m, the CPM simulation using the [Beetstra et al. \(2007\)](#) drag model
 510 again shows good agreement with the experimental data. In contrast, the MP-PIC (Barracuda)
 511 results under-predict both the upward particle velocity in the spout and the downward particle
 512 velocity in the annulus. The under-prediction of particle velocity in the MP-PIC (Barracuda)
 513 simulations can be attributed to the particle stress model used. As shown in Fig. 10, MP-
 514 PIC (Barracuda) predicts a weaker gas-jet penetration into the bed compared with CPM. In
 515 addition, small bubbles are observed near the side walls in the MP-PIC (Barracuda) simulation,
 516 whereas such structures are absent in the CPM simulation. Based on these observations, the
 517 CPM simulation without smoothing using the [Beetstra et al. \(2007\)](#) drag model provides the
 518 best overall agreement with the experimental data.

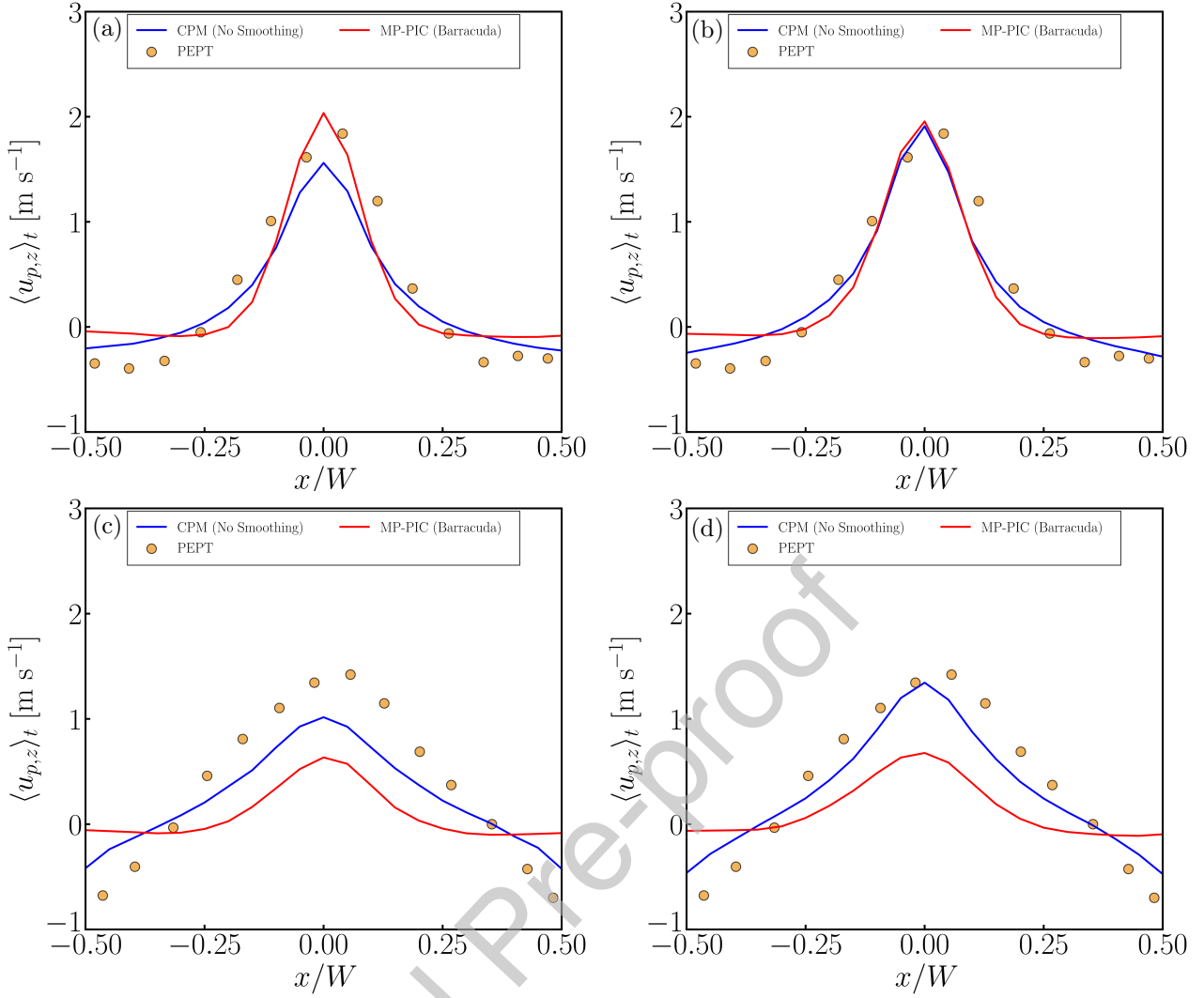


Fig. 9: Comparison of the time-averaged vertical particle velocity obtained from CPM and MP-PIC (Barracuda) with the PEPT measurements of Link et al. (2008) in the single-spout fluidized bed. (a, b) $z = 0.15$ m and (c, d) $z = 0.25$ m. Left column: simulations with Wen and Yu (1966) drag model and right column: simulations with Beetstra et al. (2007) drag model.

4.2.3. Effect of different smoothing characteristic sizes (δ_f) on CPM simulations

To examine the effect of the smoothing characteristic size on CPM predictions for the single-spout fluidized bed, simulations were performed without smoothing and with $\delta_f = 3d_p$, $5d_p$, $7d_p$, and $10d_p$. We carried out a CFD-DEM simulation, providing a more detailed reference for assessing the CPM results. To ensure consistency with the CPM simulations, particle rotation was not included in the CFD-DEM simulation.

Time-averaged particle velocity and volume fraction profiles

Fig. 11 indicates the time-averaged vertical particle velocity predicted by CFD-DEM and CPM simulations with different δ_f values, together with the experimental data of Link et al. (2008). At $z = 0.15$ m, the particle velocity in the spout region decreases as δ_f increases.

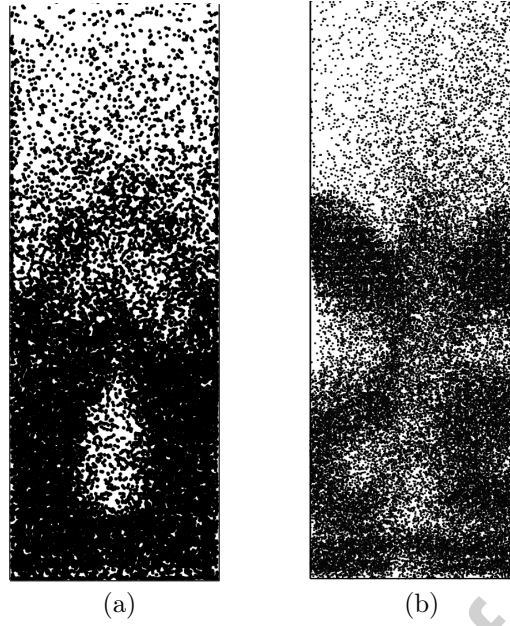


Fig. 10: Instantaneous particle distribution at $t = 15$ s from (a) CPM and (b) MP-PIC (Barracuda) in the single-spout fluidized bed.

This is because the spout channel has a cross-section of only $5.4d_p \times 2.7d_p$, while all smoothing characteristic lengths considered are larger than the spout width. As a result, the spout channel is excessively smoothed, which weakens the predicted jet penetration, as also shown in Fig. 12. However, the downward particle velocity in the annulus is less affected by δ_f than the velocity in the spout. At $z = 0.15$ m, the RMSE values relative to the experimental data for CFD-DEM and CPM without smoothing, and CPM with $\delta_f = 3d_p, 5d_p, 7d_p$, and $10d_p$ are 0.111, 0.185, 0.212, 0.311, 0.403, and 0.534, respectively. The CPM simulation without smoothing shows good agreement with both the CFD-DEM results and the experimental data. At $z = 0.25$ m, a similar trend is observed: the particle velocity decreases with increasing δ_f . At $z = 0.25$ m, the RMSE values relative to the experimental data for CFD-DEM and CPM without smoothing, and CPM with $\delta_f = 3d_p, 5d_p, 7d_p$, and $10d_p$ are 0.098, 0.231, 0.239, 0.254, 0.311, and 0.444, respectively. The CPM simulation without smoothing provides the closest agreement with the CFD-DEM results and the experimental data.

Fig. 12 shows the time-averaged particle volume fraction profiles obtained from the CFD-DEM and CPM simulations with different δ_f values for the single-spout fluidized bed. In the CFD-DEM simulation, a dilute spout channel forms at the center of the bed, while the dense annulus region is located near the side walls. A dilute fountain region is also observed above the bed surface. The CPM results show that increasing the smoothing filter size beyond $3d_p$ causes the central spout channel to disappear. Fig. 13 presents the laterally and time-averaged particle volume fraction along the bed height for the CFD-DEM and CPM simulations with

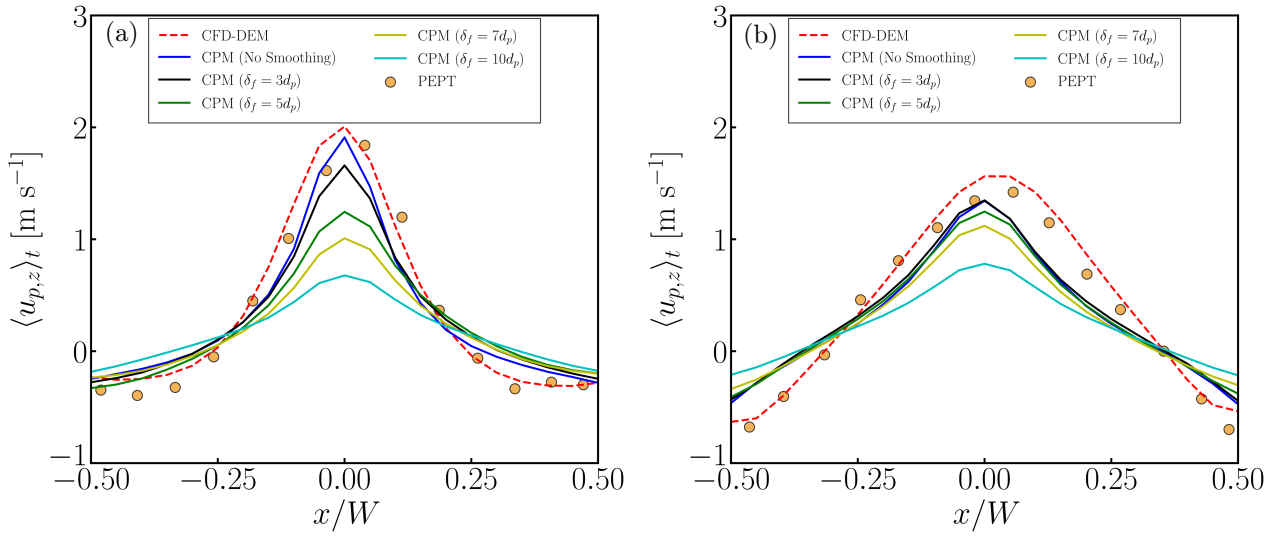


Fig. 11: Comparison of the time-averaged vertical particle velocity obtained from CPM and CFD-DEM using Beetstra et al. (2007) drag model with the PEPT measurements of Link et al. (2008) in the single-spout fluidized bed at various δ_f values. (a) $z = 0.15$ m and (b) $z = 0.25$ m.

different δ_f values. Below $z = 0.2$ m, the CPM simulations under-predict the particle volume fraction compared to CFD-DEM, and this under-prediction becomes stronger as δ_f increases. Between $z = 0.2$ m and $z = 0.3$ m, the CPM results are close to the CFD-DEM predictions. Above $z = 0.3$ m, the CPM simulation without smoothing shows the best agreement with the CFD-DEM results.

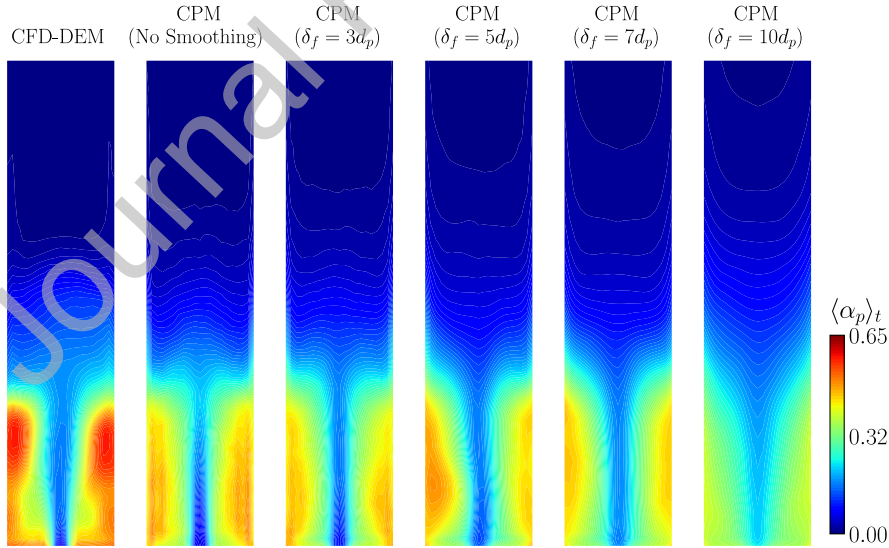


Fig. 12: The time-averaged particle volume fraction profiles obtained from CFD-DEM and CPM simulations using various δ_f values in the single-spout fluidized bed.

Particle mixing

The mixing evolution in the single-spout fluidized bed, quantified using the NDM, is shown in Fig. 14. As discussed earlier, the Lacey index is not well suited for spouted and fluidized

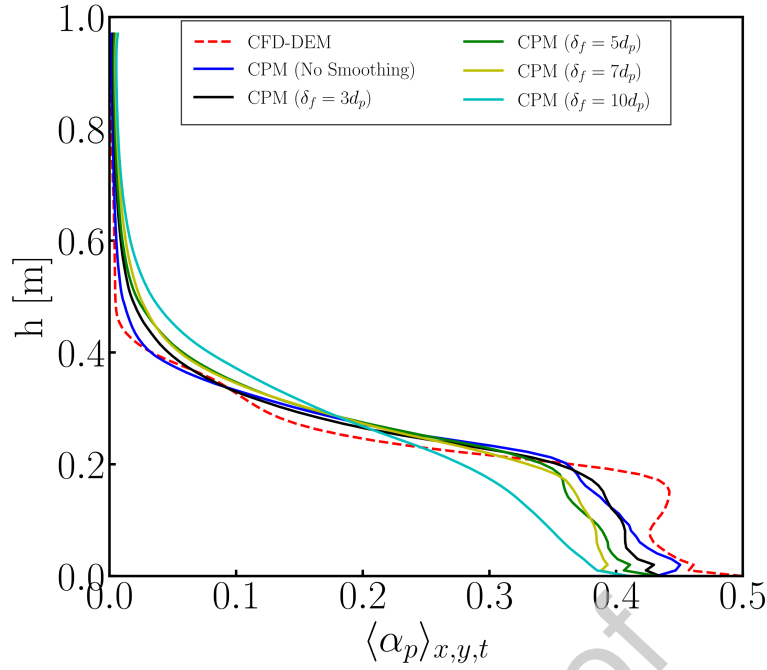


Fig. 13: The laterally and time-averaged particle volume fraction along the bed height from CFD-DEM and CPM simulations with different δ_f values in the single-spout fluidized bed.

beds; therefore, its results are not reported here. Similar to the observations for the fluidized
 bed, mixing occurs more rapidly in the CPM simulations than in the CFD-DEM simulations,
 as also evident from Fig. 15. Moreover, the CPM results indicate a slight increase in the mixing
 rate with increasing δ_f .

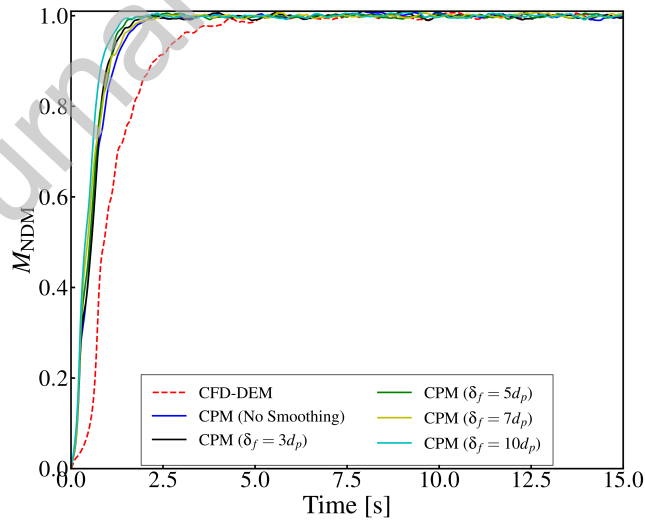


Fig. 14: Comparison of the mixing degree obtained using Nearest distance method (NDM) from CFD-DEM and CPM simulations with different δ_f values in the single-spout fluidized bed.

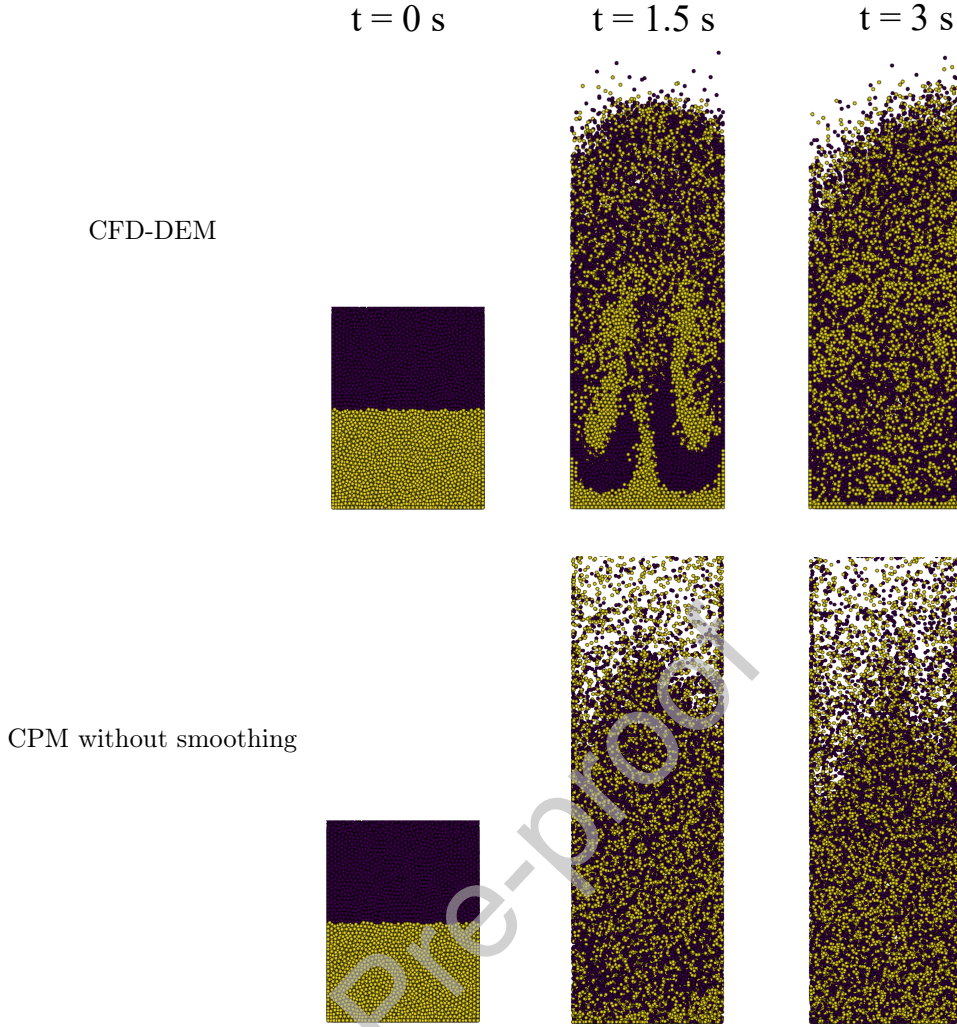


Fig. 15: Comparison of the mixing of the particles obtained from CFD-DEM and CPM without smoothing at different simulation instants in the single-spout fluidized bed.

4.3. Triple-spout fluidized bed of [van Buijtenen et al. \(2011\)](#)

4.3.1. Simulation settings

Experimental data from the triple-spout fluidized bed study of [van Buijtenen et al. \(2011\)](#) were employed to assess the performance of the CPM. The corresponding simulation parameters and material properties are summarized in Table 4, while the bed geometry is presented in Fig. 16. The computational grid size was approximately $1.67d_p$ to resolve the spouts in the x -direction, resulting in $87 \times 4 \times 360$ cells in the x -, y -, and z -directions, respectively. This grid spacing size was chosen based on the grid independence studies of [Schneiderbauer et al. \(2012\)](#) and [Yang et al. \(2016\)](#). A total of 107000 Geldart D particles was used in the simulations. Each simulation was conducted for 20 s to achieve a statistically steady state, and the statistics were averaged from 5 s to 20 s. No-slip boundary condition was imposed on the gas phase at the walls. At the spout and background inlets, a uniform gas velocity was specified, whereas atmospheric pressure was applied at the top outlet. The computational time for 1 s of simulation on 16-core

574 CPU with 2.6 GHz frequency in case of CPM and CFD-DEM simulations was 2767 s and 9770
 575 s, respectively.

Table 4: Simulation parameters related to triple-spout fluidized bed of [van Buijtenen et al. \(2011\)](#).

Property	Value	Unit
d_p	3	mm
μ_f	1.8×10^{-5}	$\text{kg m}^{-1} \text{s}^{-1}$
ρ_f	1.2	kg m^{-3}
ρ_p	2505	kg m^{-3}
g	9.81	m s^{-2}
e_{p-p}	0.8	-
μ_{p-p}	0.3	-
α_{QS}	0.1	-
α_p^{max}	0.65	-
α_{int}	0.1	-
α_{inert}	0.04	-
k	1000	N m^{-1}
Δt	0.00025	s

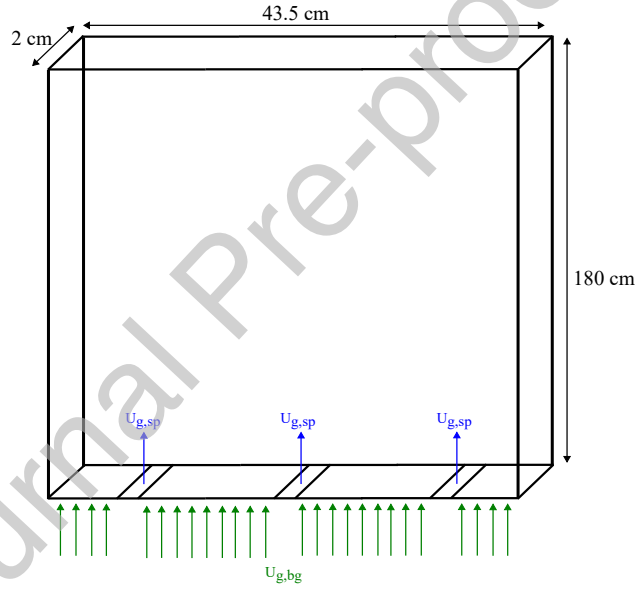


Fig. 16: The geometry of triple-spout fluidized bed of [van Buijtenen et al. \(2011\)](#). The $U_{g,sp}$ is 43.8 m s^{-1} and $U_{g,bg}$ is 2.3 m s^{-1} .

576 4.3.2. Validation results

577 Fig. 17 compares the time-averaged particle velocity predicted by MP-PIC (Barracuda)
 578 and CPM with $\delta_f = 5d_p$, using [Wen and Yu \(1966\)](#) drag model and [Beetstra et al. \(2007\)](#)
 579 drag model, against the Particle Image Velocimetry (PIV) and PEPT measurements of [van](#)
 580 [Buijtenen et al. \(2011\)](#). At $z = 0.02 \text{ m}$, both MP-PIC (Barracuda) and CPM overpredict
 581 the particle velocity in the spout regions relative to the experimental data. At $z = 0.02 \text{ m}$,
 582 the RMSE values relative to the PIV data for CPM ($\delta_f = 5d_p$) and MP-PIC are 0.090 and
 583 0.101, respectively, with the [Wen and Yu \(1966\)](#) drag model, and 0.155 and 0.168, respectively,

with the [Beetstra et al. \(2007\)](#) drag model. It can be seen from the RMSE values that the discrepancies are smaller for CPM compared to the experiments. At $z = 0.05$ m, the CPM results show good agreement with the measurements, with [Wen and Yu \(1966\)](#) drag model providing the closest match. The RMSE values relative to the PIV data for CPM ($\delta_f = 5d_p$) and MP-PIC are 0.106 and 0.204, respectively, with the [Wen and Yu \(1966\)](#) drag model, and 0.114 and 0.198, respectively, with the [Beetstra et al. \(2007\)](#) drag model. At $z = 0.1$ m, the experiments clearly show that the spouts have merged, whereas this behavior is not captured by the MP-PIC (Barracuda) simulations. In contrast, the CPM results reproduce the spout merging to a greater extent, with [Beetstra et al. \(2007\)](#) drag model showing slightly better merging behavior than [Wen and Yu \(1966\)](#) drag model. The RMSE values relative to the PIV data for CPM ($\delta_f = 5d_p$) and MP-PIC are 0.164 and 0.245, respectively, with the [Wen and Yu \(1966\)](#) drag model, and 0.158 and 0.253, respectively, with the [Beetstra et al. \(2007\)](#) drag model. The inability of MP-PIC (Barracuda) to capture spout merging is attributed to the particle stress model used in Barracuda (Eq. (39)), which generates a large particle stress that prevents the spouts from merging, as is also evident from Fig. 18. Nevertheless, among the CPM cases, [Wen and Yu \(1966\)](#) drag model was selected for the subsequent simulations because it provides the overall best agreement with the experimental data.

4.3.3. Effect of different smoothing characteristic sizes (δ_f) on CPM simulations

To investigate the effect of the smoothing characteristic size on the CPM simulation of the triple-spout fluidized bed, we performed simulations without smoothing and with $\delta_f = 3d_p$, $5d_p$, $7d_p$, and $10d_p$. Furthermore, based on the validation results, we carried out a CFD-DEM simulation employing the [Wen and Yu \(1966\)](#) drag model and $\delta_f = 5d_p$ to further assess the CPM predictions against a more detailed simulation approach. To remain in line with the CPM simulations, particle rotation was not included in the CFD-DEM simulations.

Time-averaged particle velocity and volume fraction profiles

Fig. 19 presents the time-averaged vertical particle velocity profiles obtained from CFD-DEM and CPM simulations with different values of δ_f , together with the experimental data of [van Buijtenen et al. \(2011\)](#). At $z = 0.02$ m, the particle velocity decreases as δ_f increases. This behavior may be attributed to the smoothing effect, which reduces jet penetration into the bed as also discussed around Fig. 11 for the single-spout fluidized bed. In addition, the CPM simulations without smoothing and with $\delta_f = 3d_p$ overpredict the particle velocity relative to the experiments, whereas the CPM simulation with $\delta_f = 10d_p$ underpredicts it. The RMSE

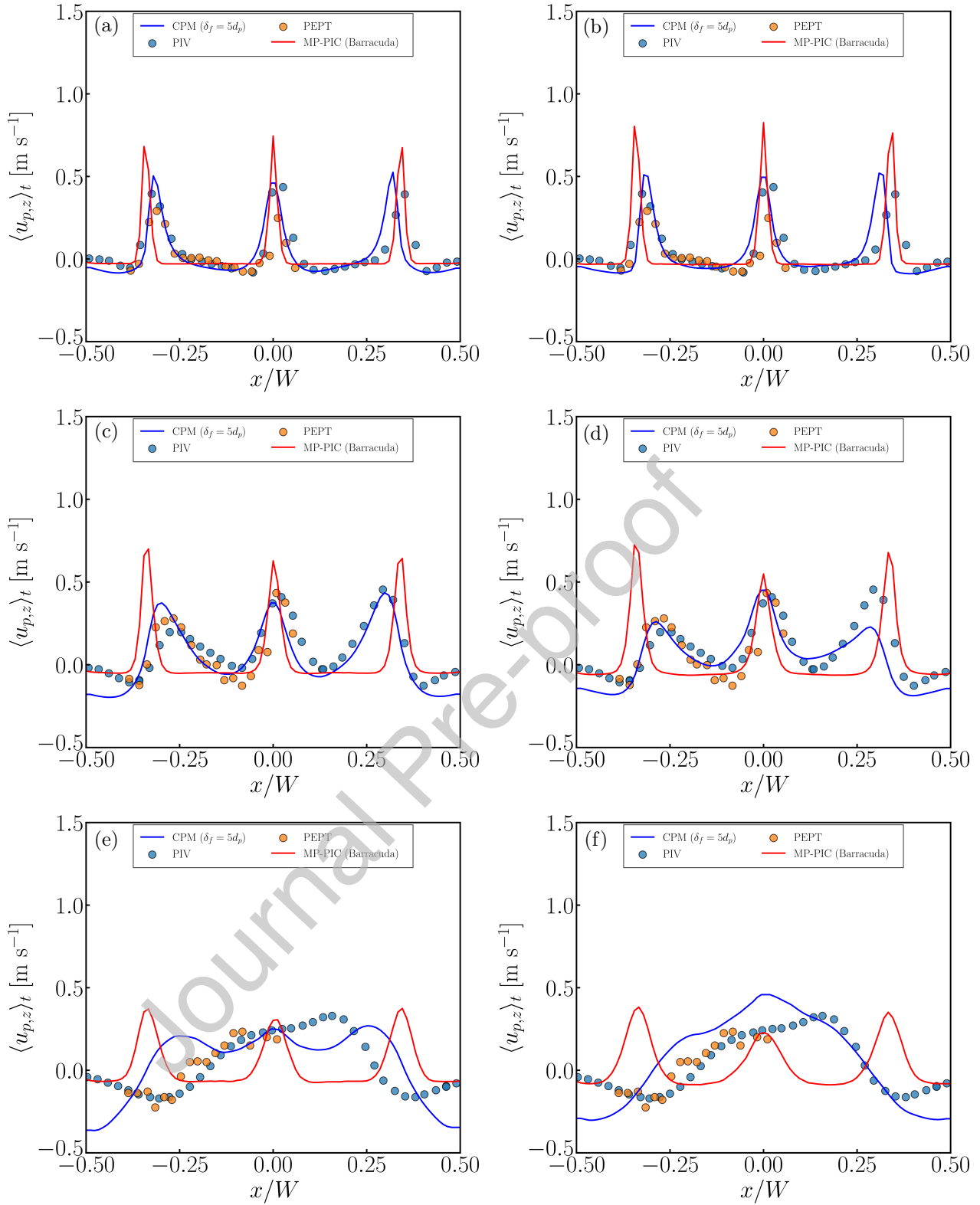


Fig. 17: Comparison of the time-averaged vertical particle velocity obtained from CPM and MP-PIC (Barracuda) with the PIV and PEPT measurements of [van Buijtenen et al. \(2011\)](#) in the triple-spout fluidized bed. (a, b) $z = 0.02$ m, (c, d) $z = 0.05$ m, and (e, f) $z = 0.1$ m. Left column: simulations with [Wen and Yu \(1966\)](#) drag model and right column: simulations with [Beetstra et al. \(2007\)](#) drag model.

values relative to the PIV data for CFD-DEM and CPM without smoothing, and CPM with $\delta_f = 3d_p, 5d_p, 7d_p$, and $10d_p$ are 0.085, 0.158, 0.119, 0.090, 0.142, and 0.128, respectively. Among the CPM cases, the simulation with $\delta_f = 5d_p$ shows the closest agreement with the

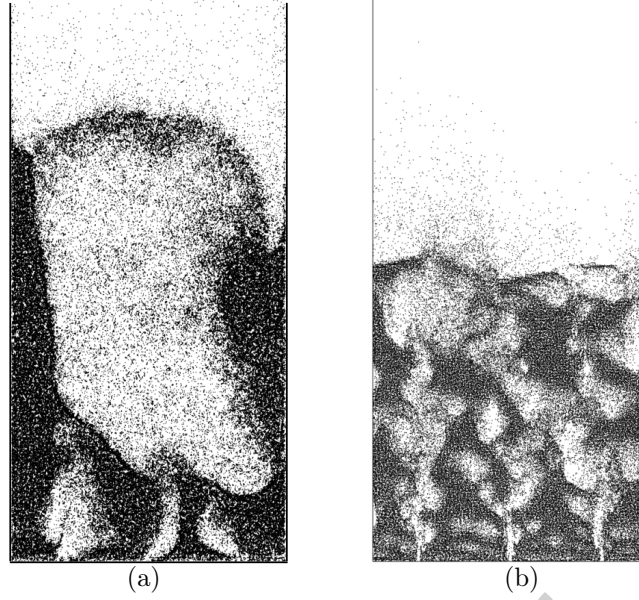


Fig. 18: Instantaneous particle distribution at $t = 20$ s from (a) CPM and (b) MP-PIC (Barracuda) in the triple-spout fluidized bed.

CFD-DEM results. At $z = 0.05$ m, the CPM simulations without smoothing and with $\delta_f = 3d_p$ again overpredict the particle velocity. In contrast, the CPM simulations with $\delta_f = 7d_p$ and $10d_p$, as well as the CFD-DEM simulation, underpredict the particle velocity in the right and central spout channels. Near the side walls, the CFD-DEM results are in better agreement with the experimental data, which may be due to the explicit resolution of individual particle-wall collisions in this approach. The discrepancy between CPM simulations and experimental results near the walls arises from the treatment of particle-particle interactions. In CPM, these interactions are represented using a closure model. Near the walls, particles accumulate and form a quasi-static region, where the stress closure model cannot capture particle interactions as accurately as CFD-DEM, which resolves individual particle contacts. In particular, the stress model in CPM is similar to fluids, where there is no shear stress in the case of zero strain, which is in contrast to particle flows supporting shear even though the particles are at rest. Therefore, the observed discrepancies in CPM are not caused by its treatment of particle-wall contacts. The RMSE values relative to the PIV data for CFD-DEM and CPM without smoothing, and CPM with $\delta_f = 3d_p$, $5d_p$, $7d_p$, and $10d_p$ are 0.124, 0.229, 0.153, 0.106, 0.128, and 0.119, respectively. At $z = 0.1$ m, it is evident that spout merging does not occur in the CPM simulations without smoothing or with $\delta_f = 3d_p$. However, as δ_f increases, the degree of spout merging becomes more pronounced. The CFD-DEM simulation shows the closest agreement with the experimental data, particularly in the central region of the bed. The RMSE values relative to the PIV data for CFD-DEM and CPM without smoothing, and CPM with $\delta_f = 3d_p$, $5d_p$, $7d_p$, and $10d_p$ are 0.116, 0.326, 0.260, 0.164, 0.165, and 0.151, respectively.

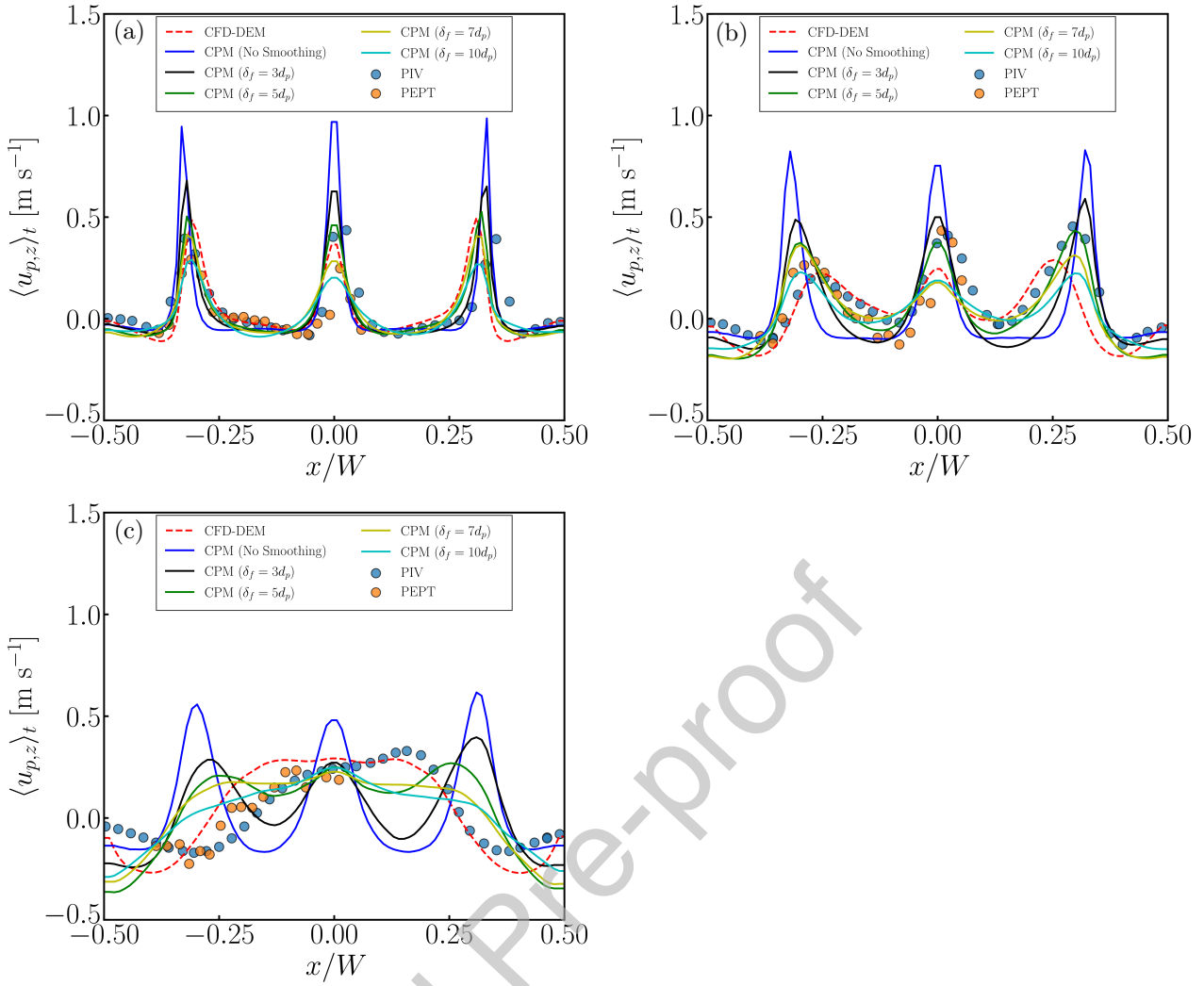


Fig. 19: Comparison of the time-averaged vertical particle velocity obtained from CPM and CFD-DEM using Wen and Yu (1966) drag model with the PIV and PEPT measurements of van Buijtenen et al. (2011) in the triple-spout fluidized bed at various δ_f values. (a) $z = 0.02$ m, (b) $z = 0.05$ m, and (c) $z = 0.1$ m.

Fig. 20 shows the time-averaged particle volume fraction profiles obtained from the CFD-DEM and CPM simulations. The results clearly demonstrate the strong influence of the smoothing characteristic size on the CPM predictions. In the CPM simulations without smoothing and with $\delta_f = 3d_p$, the spouts do not merge at the same height as in the CFD-DEM results. In our previous work (Esgandari et al., 2023), we showed using TFM that spout merging is sensitive to the particle stress. Similar to CPM, TFM relies on a continuum particle stress closure, and excessively large particle stresses can prevent the spouts from merging. In CPM, smoothing reduces sharp particle stress gradients and lowers the particle stress in the region between the spouts, thereby promoting their merging. Therefore, the observed merging is not a numerical diffusion effect caused by the grid size, which is relatively small ($1.67d_p$). Instead, it reflects a limitation of continuum particle stress models, which can predict unrealistically large particle stresses in the absence of smoothing. By contrast, in CFD-DEM, the particle

stress is determined from explicitly resolved physical contact interactions. It can also be seen that for $\delta_f = 10d_p$, the particles located between the spouts in the CFD-DEM results are no longer present in the CPM prediction, indicating that this characteristic size leads to excessive smoothing of the fields. In addition, the CPM simulations appear to predict larger bubble sizes than CFD-DEM, as reflected by the thinner dense particle layers near the side walls in CPM. Among the CPM cases, the simulation with $\delta_f = 5d_p$ shows the closest agreement with CFD-DEM.

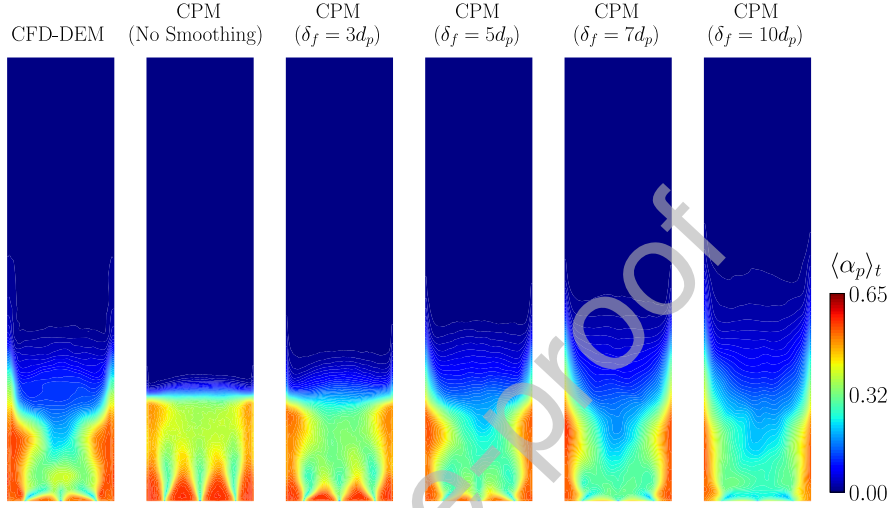


Fig. 20: The time-averaged particle volume fraction profiles obtained from CFD-DEM and CPM simulations using various δ_f values in the triple-spout fluidized bed.

Fig. 21 presents the laterally and time-averaged particle volume fraction profiles as a function of bed height for the CFD-DEM and CPM simulations with different values of δ_f . At heights below approximately 0.025 m, the particle volume fraction decreases as δ_f increases, indicating the formation of larger bubbles in the CPM simulations. In addition, as already observed in the particle volume fraction profiles in Fig. 20, the bed height, defined as the elevation at which bubbles erupt, increases with increasing δ_f . A good agreement between CFD-DEM and the CPM simulation with $\delta_f = 5d_p$ is observed near the bottom of the bed. However, in the range $z = 0.05$ -0.3 m, CFD-DEM predicts a denser particle phase than CPM. Above this region, the difference between CFD-DEM and CPM with $\delta_f = 5d_p$ becomes smaller, and both approaches predict nearly the same bed height. This is also consistent with the visual comparison in Fig. 20.

Particle mixing

The mixing degree over time in the triple-spout fluidized bed, evaluated using the NDM, is shown in Fig. 22. The results show that the smoothing characteristic size has an important

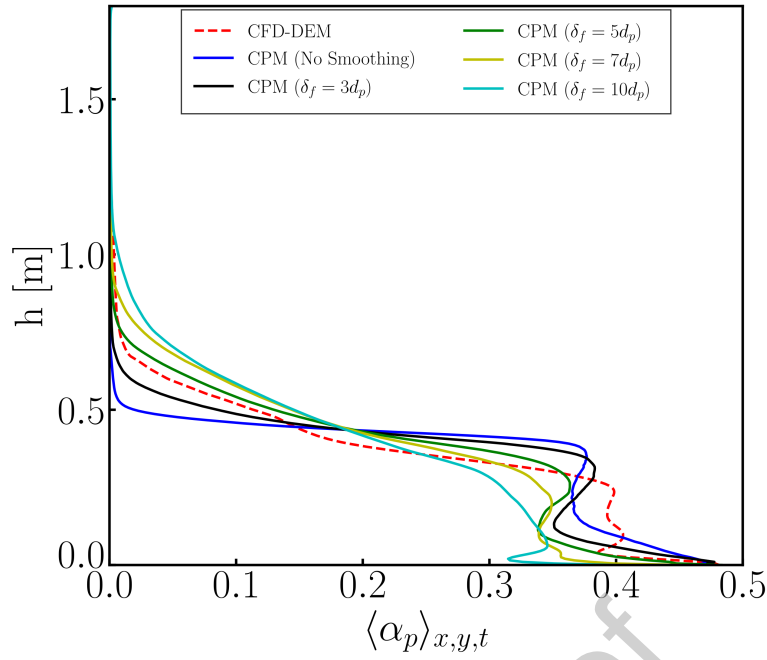


Fig. 21: The laterally and time-averaged particle volume fraction along the bed height from CFD-DEM and CPM simulations with different δ_f values in the triple-spout fluidized bed.

effect on the predicted mixing behavior. As δ_f increases, mixing occurs faster in the CPM simulations. The CPM simulation without smoothing predicts the slowest mixing because the jets do not merge at lower bed heights, which reduces the mixing rate compared with the smoothed CPM cases, as shown in Fig. 23. Consistent with the observations for the single-spout fluidized bed and the conventional fluidized bed, the CPM simulations with smoothing predict faster mixing than the CFD-DEM simulations, as also evident in Fig. 23. Overall, the CPM results indicate that increasing δ_f enhances the mixing rate in the triple-spout fluidized bed.

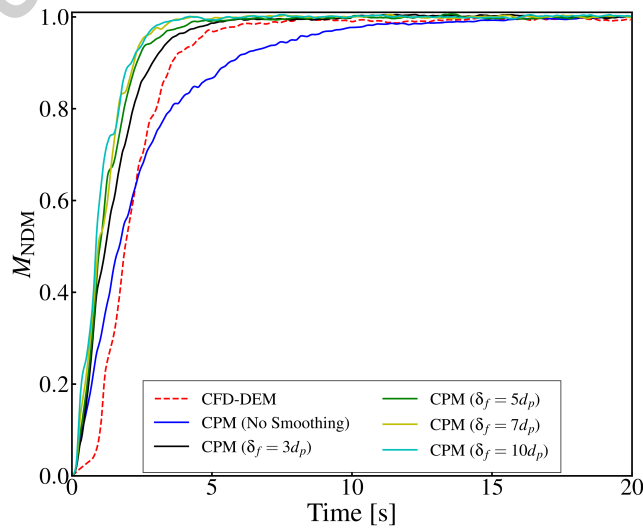


Fig. 22: Comparison of the mixing degree obtained using Nearest distance method (NDM) from CFD-DEM and CPM simulations with different δ_f values in the triple-spout fluidized bed.

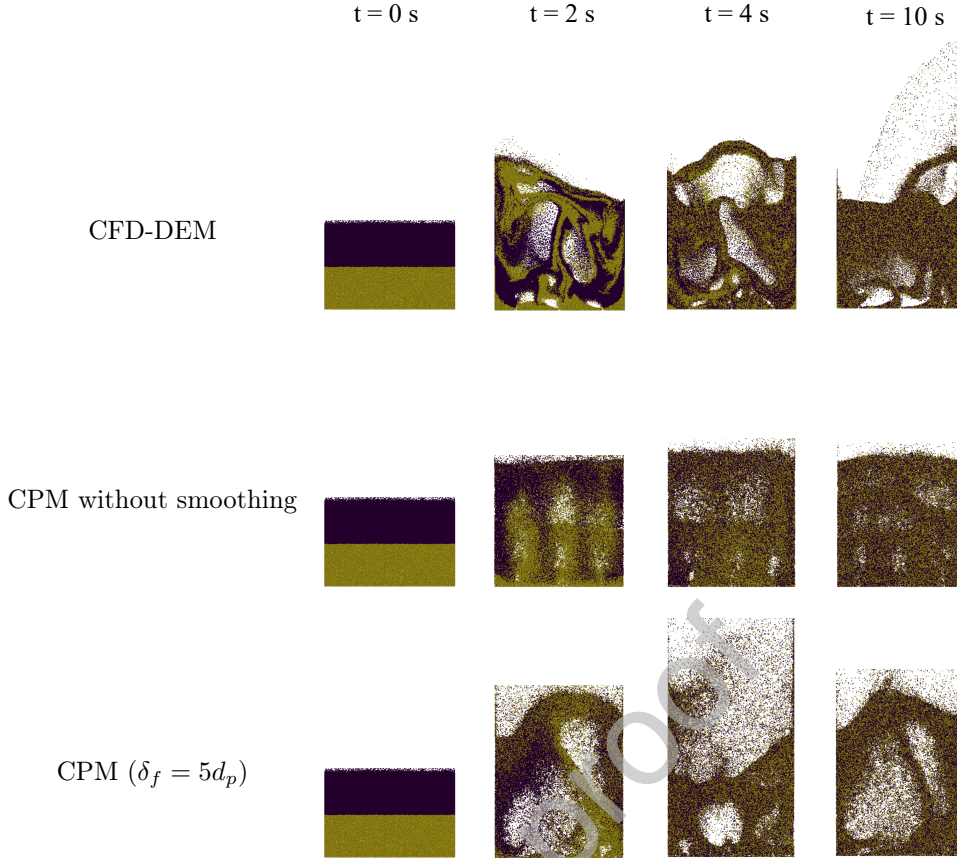


Fig. 23: Comparison of the mixing of the particles obtained from CFD-DEM, CPM without smoothing, and CPM using $\delta_f = 5d_p$ at different simulation instants in the triple-spout fluidized bed.

5. Conclusion and outlook

In this work, we presented a new CPM implementation based on a face interpolation approach. We compared CPM, MP-PIC (Barracuda), and CFD-DEM in spout-fluidized and fluidized bed cases using experimental data. In particular, we validated the simulations against time-averaged particle velocity data and found that CPM agrees well with the experiments, while MP-PIC (Barracuda) shows larger deviations. By comparing two drag models, one obtained from experiments and one derived from DNS simulations, we showed that the incorrect behavior of MP-PIC (Barracuda) simulations does not result from the choice of drag model. Instead, it stems from the simplified particle stress model, which depends only on the particle fraction and includes only isotropic particle pressure. In contrast, the particle stress model used in our CPM simulations includes isotropic particle pressure as well as viscous and frictional particle stresses. We showed that using a particle stress model that accounts for all these stress contributions leads to good agreement with both experiments and CFD-DEM data.

We examined how smoothing particle data fields affects CPM simulations. Studying the effect of the smoothing characteristic size showed that the most appropriate value depends on the particle size, grid size, and specific features of the system. In homogeneous fluidized-

bed systems, the smoothing characteristic size used in this study, $7d_p$, is larger than the grid size, $4.6d_p$, while remaining sufficiently small to resolve the smallest bubbles. In our previous work (Esgandari and Schneiderbauer, 2025), we showed that this smoothing characteristic size produces grid-independent results for unbounded homogeneous fluidization systems. Therefore, for homogeneous systems such as bubbling fluidized beds, a smoothing characteristic length of approximately 1.5 times the grid size is recommended. For the single-spout fluidized bed, resolving the distinct spout channel is more important. Based on the spout channel cross-section of $5.4d_p \times 2.7d_p$, the smoothing characteristic sizes considered in this study are larger than the channel width of $2.7d_p$, which causes the spout channel to be smeared. Therefore, smoothing is not recommended when the spout channel width is smaller than the smoothing characteristic length. For the triple-spout fluidized bed, as shown in our previous work (Esgandari et al., 2023), the correct system behavior depends strongly on the particle stress in the regions between the spouts, and smoothing is therefore required. For this system, a smoothing characteristic length of $7d_p$, corresponding to approximately three grid cells, is recommended.

In addition, we studied particle mixing using two mixing indices: a grid-based method, namely the Lacey index, and a distance-based method, namely the Nearest Distance Method. We showed that the Lacey index is not suitable for evaluating the degree of mixing in fluidized and spout-fluidized beds because these systems contain dense and dilute regions at the same time. In particular, dilute regions create grid cells with very low particle concentrations, which can distort the cell-based statistics and lead to artificial behavior in the Lacey index. Therefore, we selected the Nearest Distance Method to compare the mixing evolution between CPM and CFD-DEM simulations. We found that although CPM agrees well with CFD-DEM in terms of time-averaged particle velocity and volume fraction, it predicts a faster mixing rate than CFD-DEM in all cases studied in this paper. In addition, it was shown that CPM is $8\times$, $2.8\times$, and $3.5\times$ faster than CFD-DEM in case of fluidized bed, single-spout fluidized bed, and triple-spout fluidized bed simulations, respectively.

This work provides essential insights into the application of CPM compared with MP-PIC and CFD-DEM, particularly for industrial-scale chemical engineering systems where CFD-DEM is computationally prohibitive. We also revealed the advantage of CPM over MP-PIC in dense fluidized systems. Future studies should extend these comparisons to dilute systems, such as risers. In addition, CPM can account for polydisperse particles, and comparisons with CFD-DEM would help further extend its range of applications. Furthermore, extending the CPM model to include heat transfer and reactions could be beneficial for applications such as iron ore reduction in industrial-scale fluidized beds (Schneiderbauer et al., 2020).

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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CRedit authorship contribution statement

Behrad Esgandari: Conceptualization; Methodology; Software; Formal analysis; Investigation; Data curation; Writing-Original Draft; Writing - Review & Editing; Visualization, **Zahra Aminigarakani:** Methodology; Investigation; Resources; Data curation; Review & Editing, **Bradley Paul Ladewig:** Supervision; Project administration; Funding acquisition; Review & Editing, **Simon Schneiderbauer:** Writing – Review & Editing, Supervision, Methodology, Software, Project administration, Funding acquisition, Conceptualization

Appendix A. Influence of P^* and β parameters in the particle stress model of Harris and Crighton (1994) on MP-PIC (Barracuda) simulations

We investigated the effects of the P^* and β parameters in the particle stress model of Harris and Crighton (1994) on MP-PIC (Barracuda) simulations of the bubbling fluidized bed studied by Gopalan et al. (2016), as shown in Fig. A.1. The results indicate that varying P^* and β does not improve the MP-PIC predictions. Moreover, increasing P^* beyond 20 suppresses bubbling in the bed.

Appendix B. Effect of particle rotation in CFD-DEM simulations

Fig. B.1 compares the time-averaged axial particle velocity predicted by CFD-DEM simulations with and without particle rotation for the bubbling fluidized bed studied by Gopalan

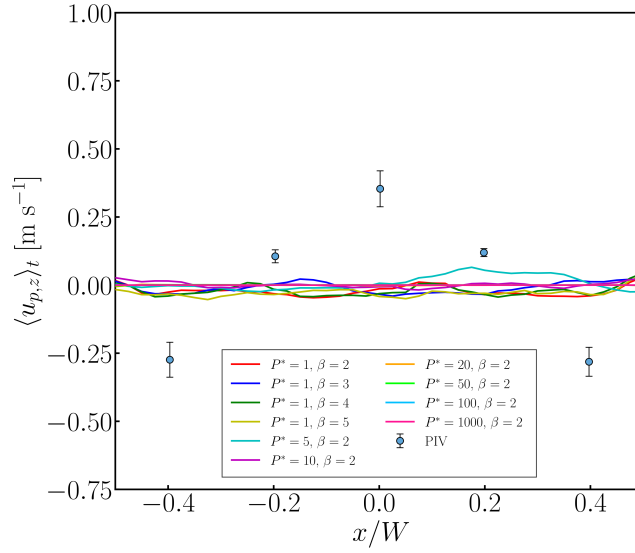


Fig. A.1: Comparison of the time-averaged vertical particle velocity obtained from MP-PIC (Barracuda) using various P^* and β parameters.

et al. (2016). Including particle rotation reduces the magnitude of the downward particle velocity in the dense near-wall regions, likely because of increased dissipation of particle momentum. In contrast, particle rotation has little influence on the velocity profile in regions farther from the walls.

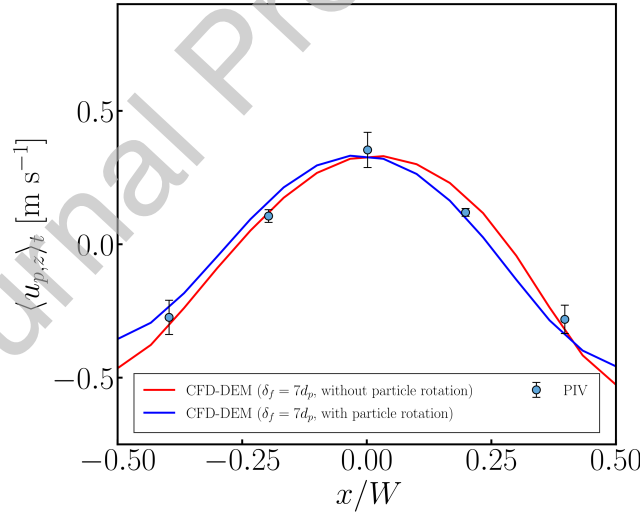


Fig. B.1: The time-averaged axial particle velocity predicted by CFD-DEM simulations with and without particle rotation.

Appendix C. Influence of the computational cell size on Lacey index predictions

To investigate the effect of computational cell size on the predicted Lacey mixing index, five different cell configurations were examined using the coarse-particle model (CPM) with $(\delta_f = 7d_p)$, as shown in Fig. C.1. The results demonstrate that the predicted Lacey index is sensitive to the selected cell size. As the cell size decreases, corresponding to an increase in the

number of computational cells, the maximum degree of mixing decreases and the magnitude of the fluctuations increases. Based on this sensitivity analysis, a grid comprising $(16 \times 5 \times 80)$ cells was selected for the evaluation of particle mixing in this study.

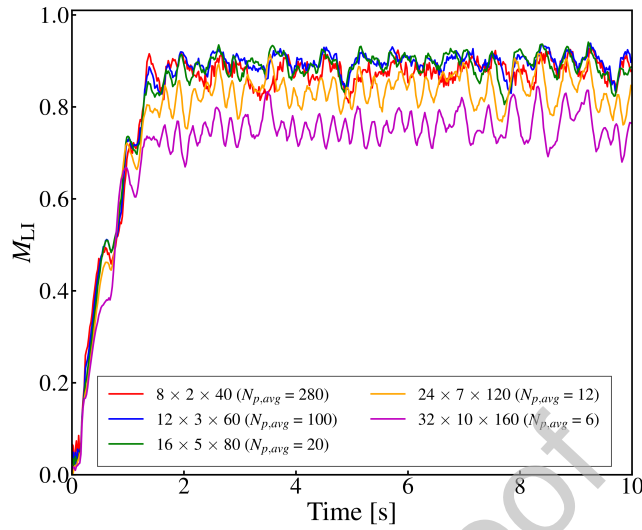


Fig. C.1: Comparison of the mixing degree in CPM ($\delta_f = 7d_p$) obtained from Lacey index using different cell sizes.

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