Numerical Investigation of Particle Preferential Concentration in Homogeneous Turbulence Using DNS

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Abstract

T his study aims to establish a quantitative relationship between particle preferential concentration and key governing variables—fluid-to-particle density ratio (ρ_f/ρ_p) and Stokes number (St_k)—in homogeneous, isotropic turbulence. Using Direct Numerical Simulations (DNS) with two-way coupling, we analyze particle-laden flows in an Eulerian-Lagrangian framework with a uniform mesh resolution of 128^3 and a particle volume fraction of 10^{-3}. The simulations isolate the effects of density ratio at a fixed Stokes number ($St = 1$) and explore the influence of varying St_k to understand the interplay between particle inertia and turbulent structures.

Results reveal a non-monotonic relationship between particle density and clustering, with maximum preferential concentration observed at $\rho_p = 500$ and reduced clustering at intermediate densities ($\rho_p = 300$). For varying Stokes numbers, clustering peaks at $St_k = 1$ and diminishes at both lower and higher values, consistent with the centrifuge effect. Correlation trends between particle number density and the Q-criterion align with theoretical expectations, showing a consistent negative relationship that supports the centrifuge effect. However, the weak magnitude of these correlations suggests that the relationship is not strongly quantifiable, highlighting the influence of additional factors such as turbulence intermittency and particle-particle interactions. Snapshots of particle distributions and Radial Distribution Function (RDF) analyses further illustrate the preferential accumulation of particles in strain-dominated regions and their avoidance of vortex cores.

These findings highlight the critical roles of particle density and inertia in modulating preferential concentration. By combining high-fidelity simulations with systematic analysis, this study advances the understanding of particle-turbulence interactions and provides a robust framework for future investigations. The study underscores the need for alternative turbulence metrics to fully capture preferential concentration mechanisms and offers a foundation for improved predictive models in applications ranging from aerosol dynamics to chemical reactor design.

Keywords: turbulence, DNS, preferential concentration, two-way coupling, particle-laden flow

I. INTRODUCTION

Particle-laden turbulent flows are ubiquitous in both natural and industrial contexts, playing an essential role in processes ranging from pollutant transport in the atmosphere to spray combustion, sediment transport, and chemical manufacturing [3], [11]. These flows involve intricate interactions between suspended particles and the turbulent eddies of a carrier fluid, resulting in a spectrum of behaviors from uniform particle dispersion to significant clustering. One of the fascinating phenomena observed in these systems is preferential concentration, wherein particles with finite inertia tend to accumulate in regions of low vorticity and high strain rate, creating clusters and voids within the flow [6], [9]. This clustering significantly impacts mixing, heat transfer, and chemical reaction rates in industrial processes, as well as sedimentation and ecological dispersal in natural environments [6].

The Stokes number (St) is a fundamental dimensionless parameter governing particle dynamics in turbulent flows and plays a crucial role in preferential concentration—the tendency of inertial particles to accumulate in specific flow regions rather than being uniformly distributed. Defined as the ratio of the particle response time to a characteristic flow timescale, typically the Kolmogorov time scale τ_k, it encapsulates the balance between inertial and drag forces acting on particles. Preferential concentration arises because particles with different inertia interact uniquely with turbulent structures. Particles with $St < 1$ closely follow fluid streamlines, behaving as tracers, while particles with $St = 1$ exhibit ballistic trajectories, largely decoupled from the carrier flow [7], [10]. Notably, when $St \approx 1$, particles exhibit optimal inertia, leading to their centrifugation out of vortex cores and preferential accumulation in strain-dominated regions. This behavior, often described as the centrifuge effect, highlights how St dictates the spatial distribution of particles and contributes to clustering phenomena in turbulence [3], [4].

Recent studies have expanded our understanding of preferential concentration by exploring how other particle properties, such as density ratio (ρ_f/ρ_p), influence clustering behavior. For instance, Monchaux et al. [9] highlighted the significance of density ratios in modulating particle-turbulence interactions, emphasizing the importance of additional mechanisms such as the sweep-stick effect, which preferentially positions particles in low-acceleration regions. Similarly, Chowdhury [3] reviewed experimental and numerical works, showing that particle clustering depends not only on (ρ_f/ρ_p) but also on Reynolds number and void fraction. These findings point to the complexity and richness of particle dynamics in turbulent flows, which are governed by an interplay of local flow features, particle properties, and external forces such as gravity.

This study quantitatively examines the influence of both the fluid-to-particle density ratio (ρ_f/ρ_p) and the Stokes number (St) on particle preferential concentration within turbulent flows. To isolate the effects of density variation on the particle preferential concentration within the turbulent structures, simulations are conducted at a fixed Stokes number at unity, while a separate analysis explores how varying St affects clustering behavior. Direct Numerical Simulations (DNS) with two-way coupling are employed to capture the complex interactions between particles and turbulence. Particle clustering is analyzed using the Q-criterion and the Radial Distribution Function (RDF), enabling a systematic evaluation of how both density ratio and Stokes number influence preferential concentration. Correlations between Particle Number Density (PND) and the Q-criterion further quantify the relationship between particle inertia and turbulent structures. By establishing these quantitative links, this study provides a more comprehensive understanding of the mechanisms governing particle dynamics in turbulence.

The results of this work contribute to the broader understanding of particle-laden flows, with potential applications in both natural and engineered systems. For instance, the insights gained could enhance the modeling of sedimentation processes in natural environments, such as rivers, as well as optimize engineered processes like spray combustion and chemical reactor design. By providing more quantifiable data on the relationship between particle dynamics and turbulence, this study facilitates the development of improved predictive models, including machine learning approaches and generalized empirical formulas that capture the effects of key variables. By bridging the gap between particle dynamics and turbulence, this study advances the foundational knowledge necessary for improving the efficiency and predictability of particle-laden flow systems.

II. Numerical Setup

A. Governing Equations

The study employs an Eulerian-Lagrangian framework to model the fluid-particle interactions. In this system, the fluid phase is described by the incompressible Navier-Stokes equations, while the particle phase is modelled using a Lagrangian approach.

The continuity equation ensures mass conservation in the fluid:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

where $\mathbf{u} = (u, v, w)$ represents the velocity field components.

The momentum equation describes the fluid motion, incorporating inertial, pressure, viscous, and external force terms:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}, \tag{2}$$

where ν is the kinematic viscosity, ρ is the fluid density, and $\mathbf{f}$ represents any external forces (e.g., gravity or electromagnetic forces).

Particles are modelled using a Lagrangian approach, which tracks individual particle positions and velocities as they move through the fluid flow.

The particle position $\mathbf{x}_p$ is governed by the following equation, which describes the motion of the particle as a function of its velocity $\mathbf{v}_p$:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \tag{3}$$

The particle velocity $\mathbf{v}_p$ evolves based on the difference between the particle velocity and the fluid velocity at the particle's location, with a relaxation time τ_p that accounts for the particle's inertia and drag forces:

$$\frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{u}(\mathbf{x}_p, t) - \mathbf{v}_p}{\tau_p}, \tag{4}$$

where $\mathbf{u}(\mathbf{x}_p, t)$ is the velocity field at the particle's location.

III. Computational Setup

A. Initialization and Boundary Conditions

Direct Numerical Simulations (DNS) of forced isotropic turbulence were conducted over a cubic domain of length 2π, with periodic boundary conditions applied in all three directions. The numerical methods and validations are based on the reference simulations by Bassenne et al. [2] and Esmaily-Moghadam and Mani [5], which use second-order accuracy in space and fourth-order accuracy in time.

A uniform mesh resolution of 128^3 grid points was used to accurately resolve the turbulence in the simulation. The velocity-pressure coupling was handled using the *PISO algorithm* within OpenFOAM, ensuring both accuracy and stability of the numerical solution. Spectral forcing at low wavenumbers was applied to sustain turbulence, preserving the homogeneity and isotropy of the flow while maintaining a stationary solution. The resolution criterion $k_{\max}\eta = 2.2$ was satisfied, and the Reynolds number based on the Taylor microscale was set to $Re_\lambda = 75$. A fixed particle volume fraction of 10^{-3} was maintained for all simulations to ensure consistency and accuracy in the DNS.

IV. Analysis Techniques

A. Correlation and Clustering Metrics

To quantitatively assess the relationship between particle clustering and turbulent flow structures, we employed multiple statistical measures.

The Normalized Correlation Coefficient R_{uv} is used to evaluate the degree of correlation between the Q-criterion, which identifies regions of coherent vortex structures, and the particle number density (PND):

$$R_{uv} = \frac{\langle (Q - \overline{Q})(PND - \overline{PND}) \rangle}{\sigma_Q \sigma_{\text{PND}}}, \tag{5}$$

where Q represents the local Q-criterion value, PND is the particle number density, and σ_Q and σ_{PND} are their respective standard deviations. A positive R_{uv} indicates that particles preferentially accumulate in vortex-dominated regions, while a negative value suggests clustering in strain-dominated regions.

The Radial Distribution Function (RDF) $g(r)$ provides a statistical measure of particle clustering by quantifying the relative probability of finding particle pairs at a given separation distance r:

$$g(r) = \frac{1}{4\pi r^2 \Delta r} \frac{N_p(r)}{\rho_p V}, \tag{6}$$

where $N_p(r)$ is the number of particle pairs separated by distance r, ρ_p is the average particle density, and V is the total volume of the domain. Values of $g(r) > 1$ indicate clustering, whereas $g(r) \approx 1$ corresponds to a uniform distribution.

V. Results and Analysis

A. Quantitative Analysis

Radial Distribution Function (RDF) results for varying fluid-to-particle density ratios (ρ_f/ρ_p) highlight the non-monotonic relationship between density and clustering. The trends demonstrate that particles tend to cluster in strain-dominated regions and avoid vortex cores, with an increased tendency as the density ratio increases. However, the RDF for intermediate densities, specifically $\rho_p = 300$, deviates from this expected behavior, suggesting unique turbulence-particle interactions at these levels.

In addition, RDF trends for varying Stokes numbers reveal how particle inertia influences spatial distribution. As Stokes number increases, particles preferentially accumulate in strain-dominated regions due to higher inertia, which affects their ability to follow the vortical motions within the turbulent structures.

The correlation between particle number density (PND) and the Q-criterion was analyzed for varying density ratios (ρ_f/ρ_p), revealing consistently negative values across all cases (Figure 3 (a)). At $St = 1$, particles are optimally responsive to turbulent structures, accumulating in strain-dominated regions while avoiding vortex cores. This centrifuge effect becomes more pronounced with increasing particle density, as higher inertia strengthens the resistance to vortical motions. However, the non-monotonic progression in the correlation suggests that localized turbulence intermittency and subtle flow-particle interactions may also influence clustering dynamics.

Furthermore, the correlation becomes more complex with varying Stokes numbers. At higher Stokes numbers ($St = 4, 8$), the particles' inertia prevents them from aligning with vortex cores, instead, they preferentially accumulate in strain-dominated regions, showing the intricate interplay between inertia, turbulence, and density ratio. The results for varying Stokes numbers can be seen in Figure 3 (b).

B. Qualitative Analysis

1) Particle Distribution Patterns: Figures 4 and 5 provide visualizations of particle distributions for different Stokes numbers and varying particle densities. The snapshots illustrate how clustering behavior evolves across different inertial regimes, with particles at lower Stokes numbers aligning more closely with turbulent vortices, while those at higher Stokes numbers accumulate more prominently in strain-dominated regions.

2) Interaction with Turbulent Structures: Particles with different Stokes numbers exhibit varying degrees of interaction with coherent vortices and strain-dominated regions. The results suggest that at lower Stokes numbers, particles are more closely aligned with vortex cores, while at higher Stokes numbers, they preferentially concentrate in the strain-dominated regions, highlighting the critical role of particle inertia in modulating these interactions.

3) Implications for Preferential Concentration: The combined findings from the RDF and correlation analyses, along with the particle distribution patterns, demonstrate that particle inertia and density ratio significantly modulate preferential concentration in turbulent flows. These results provide valuable insights into how these factors influence the clustering behavior of inertial particles, contributing to a deeper understanding of particle-turbulence interactions.

VI. Discussion

A. Varying Particle Density Ratio

The results of this study reveal the quantitative relationship between particle inertia, turbulent structures, and preferential concentration in particle-laden flows. By maintaining a fixed Stokes at unity and varying the fluid-to-particle density ratio, we observed distinct trends in how particles interact with coherent flow features such as vorticity and strain. The negative correlation between particle density and the Q-criterion underscores the fundamental mechanism of vorticity avoidance: particles with sufficient inertia are centrifuged out of vortex cores and instead accumulate in strain-dominated regions. This behavior aligns with the well-documented centrifuge effect [1], [8], where particles are expelled from regions of high rotational motion and driven into zones of flow compression and extension. Snapshots of particle distributions in Fig. 2 for different density ratios provide further insight into the clustering behavior. For Fig. 2(a) $\rho_p = 200$, clear clustering is observed, indicating that particles at this density respond

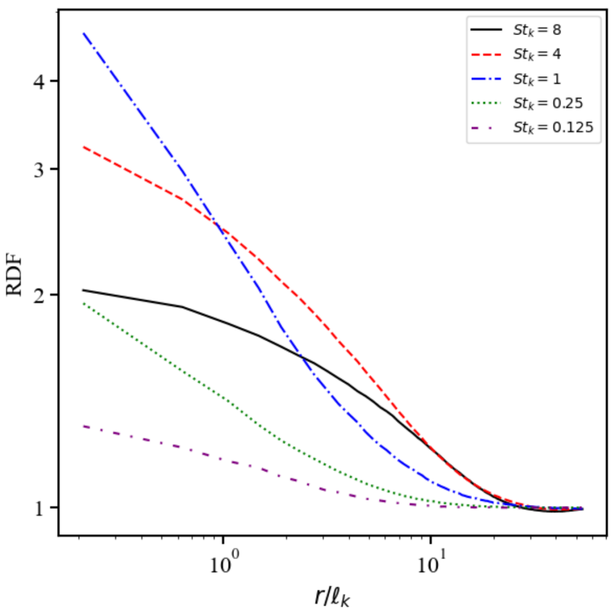

Fig. 1. Radial Distribution Functions for varying Stokes numbers, showing the influence of particle inertia on clustering behavior.

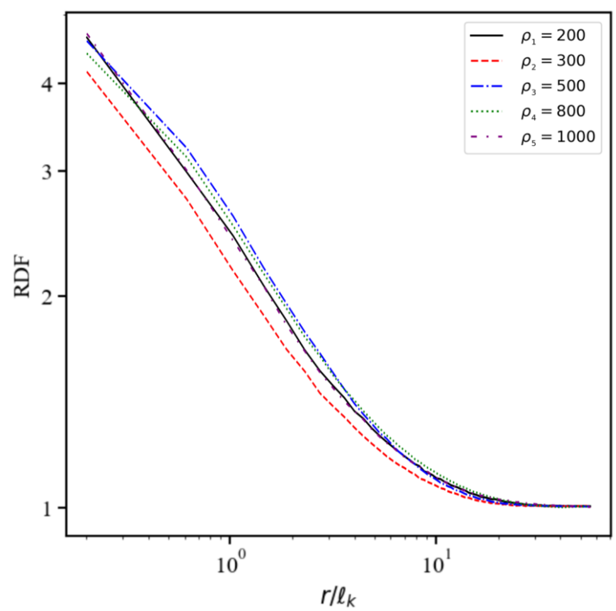

Fig. 2. Radial Distribution Functions for varying particle densities, showing how particle density ratio affects clustering.

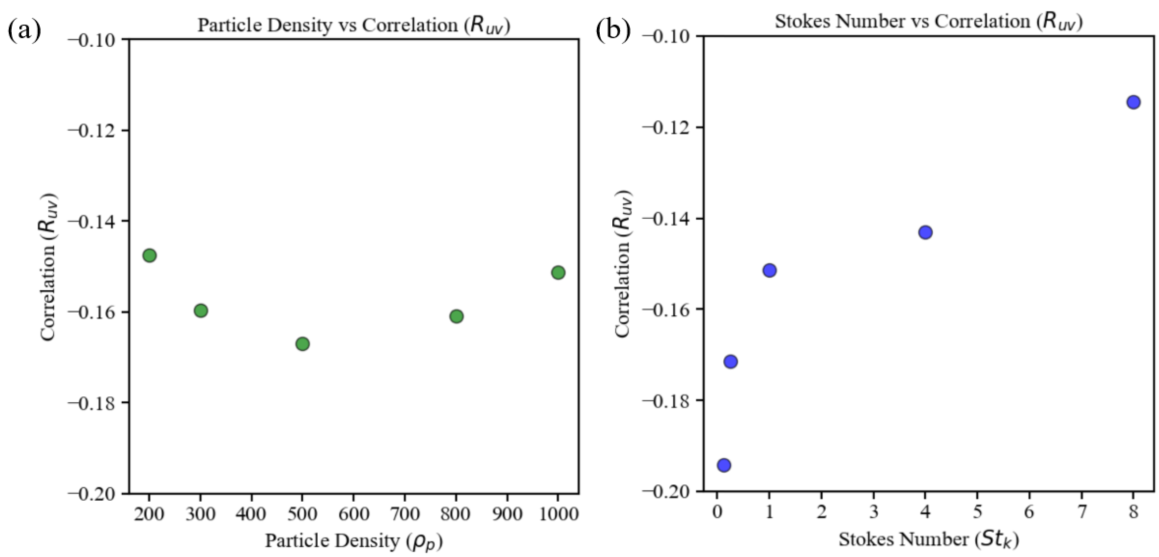

Fig. 3. Correlation between particle number density (PND) and the Q-criterion (a) for varying particle densities (b) for varying Stokes numbers.

strongly to turbulent structures. However, clustering is relatively reduced for Fig. 2(b) $\rho_p = 300$, which is consistent with the lower RDF values observed at smaller particle separations. This reduction may be attributed to transient interactions between particles and turbulence, where the particle inertia at this specific density creates a weaker coupling with flow features. For Fig. 2(c) $\rho_p = 500$, the highest level of clustering is evident, corresponding to the most negative correlation coefficient and elevated RDF values. This suggests an optimal interplay between particle inertia and turbulent strain regions. As the density increases further to Fig. 2(d) $\rho_p = 800$ and Fig. 2(e) $\rho_p = 1000$, clustering gradually increases again, though not as pronounced as at $\rho_p = 500$. This trend indicates that very high particle densities may dampen interactions with smaller turbulent scales, leading to slightly less pronounced clustering.

As the particle density increases, the enhanced inertia amplifies this effect, leading to deeper negative correlations. This is reflected in the Radial Distribution Function (RDF) analysis, which consistently demonstrated tighter clustering and elevated $g(r)$ values at smaller spatial separations for higher density ratios, with one notable exception. The RDF

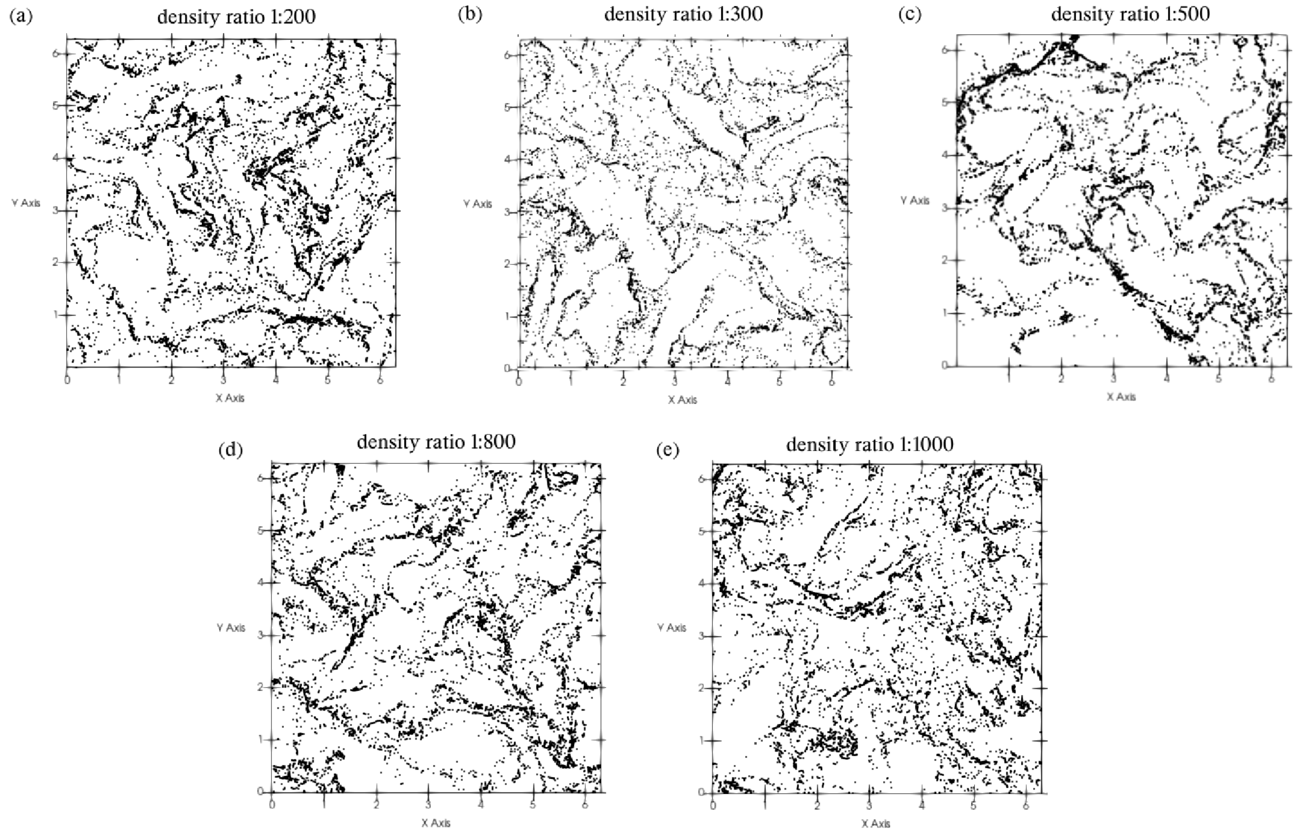

Fig. 4. Particle snapshot for varying particle densities at $St = 1$, illustrating clustering behavior across different density ratios. Slice thickness η.

trend for $\rho_p = 300$ exhibited a lower distribution at smaller particle separations compared to the other cases. This deviation suggests that particles with this specific density may interact differently with localized turbulence structures, potentially due to subtle differences in particle-fluid coupling or transient effects within the flow.

The clustering behavior highlights the role of particle-fluid interactions at a fixed response time, where particles optimize their accumulation in high-strain regions while avoiding vortex cores. This phenomenon directly relates to the balance of inertial forces and flow timescales, which are governed by the Stokes number.

The quantitative correlation analysis between particle number density and the Q-criterion, as shown in Fig. 3(a), revealed statistically significant but weak to very weak correlations across all density ratios. While these results confirm a consistent negative relationship between particle density and the Q-criterion—supporting the mechanism of vorticity avoidance—the low magnitude of the correlations suggests that the relationship is not strongly defined. This implies that while particles tend to avoid vortex cores and accumulate in strain-dominated regions, other factors, such as turbulence intermittency, transient flow structures, or particle-particle interactions, may play a more significant role in shaping particle distributions. The weak correlations highlight the complexity of particle-turbulence interactions and suggest that preferential concentration cannot be fully explained by the Q-criterion alone. These findings align with the observed clustering trends in the RDF analysis, where particle inertia and density ratios modulate clustering intensity but do not dominate the dynamics entirely.

These findings resonate with prior experimental and numerical studies, such as those by Zhang et al. (2016) and Chowdhury (2022) [3], [12], which emphasize the role of particle inertia and flow topology in driving preferential concentration.

B. Varying Stokes Number

The study extends the analysis of particle clustering and turbulence interactions by examining the impact of varying Stokes numbers at the Kolmogorov scale (St_k). Using the same metrics applied in the density ratio analysis, we observed clear trends in how particle inertia influences preferential concentration. The Radial Distribution Function (RDF) in Fig. 1 confirms the expected theoretical trend, with maximum clustering observed at $\mathrm{St}_k = 1$, followed by $\mathrm{St}_k = 4$, then $\mathrm{St}_k = 8$. The clustering effect is significantly reduced at lower Stokes numbers, with $\mathrm{St}_k = 0.25$ exhibiting minimal

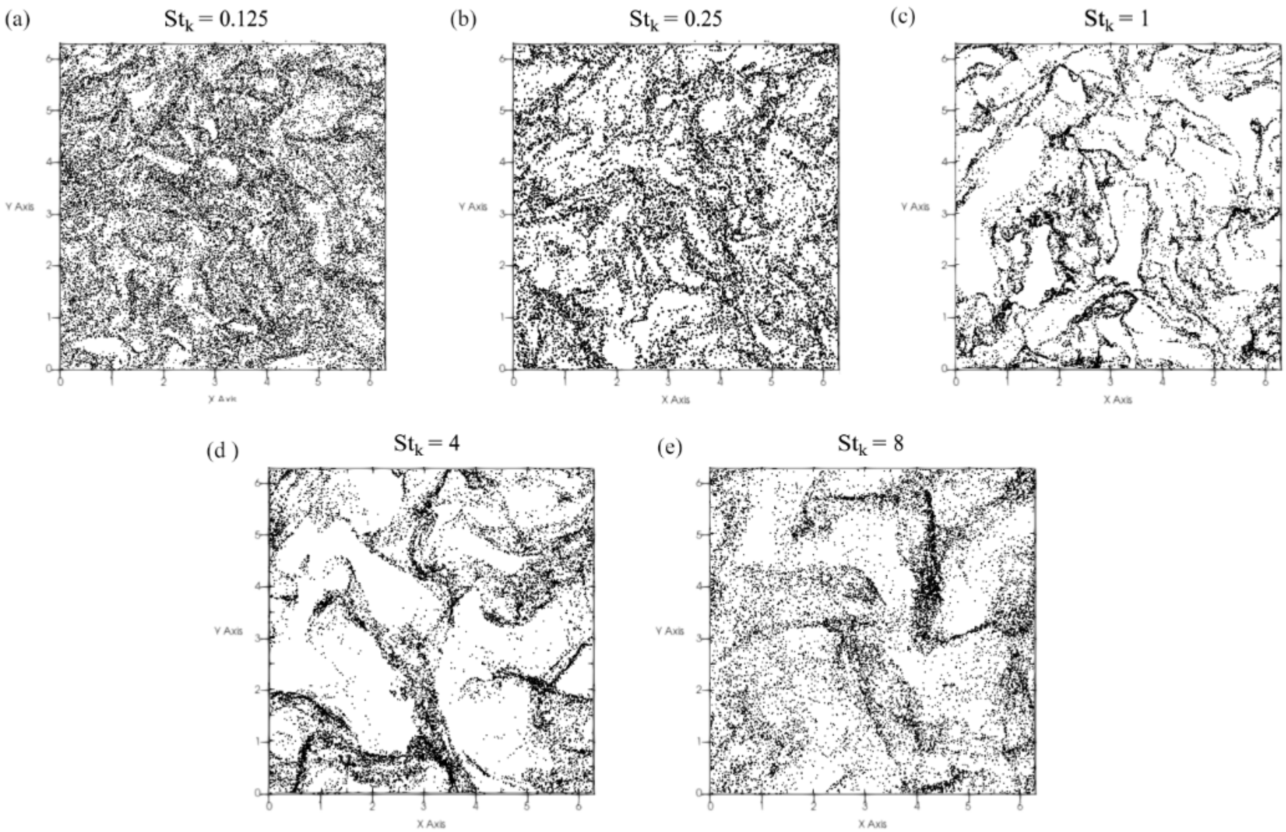

Fig. 5. Particle snapshot for varying Stokes numbers at $\rho_p = 1000$, showing how particle preferential concentration is influenced by inertia. Slice thickness η.

clustering and $\mathrm{St}_k = 0.125$ displaying the weakest preferential concentration.

Snapshots of particle distributions in Fig. 5 further illustrate these trends. At $\mathrm{St}_k = 1$, particles accumulate most strongly in high-strain regions while avoiding vortex cores, demonstrating the optimal balance between inertia and turbulent flow structures. As St_k increases to 4 and 8, clustering remains prominent but gradually diminishes, suggesting that particles with higher inertia interact less with small-scale turbulence and instead respond to larger-scale flow features. Conversely, at very low St_k values (0.125 and 0.25), clustering is nearly absent, indicating that these particles are strongly coupled to the fluid and distribute more uniformly within the turbulent field.

The quantitative correlation analysis between particle number density and the Q-criterion, shown in Fig. 3(b), reveals a weak negative correlation across all St_k values, with correlation coefficients ranging from -0.1942 to -0.1144. This confirms the expected trend that inertial particles tend to be expelled from vortex cores due to centrifugal forces. However, the decreasing magnitude of correlation as St_k increases suggests that highly inertial particles interact with turbulence in a more stochastic manner, becoming less sensitive to small-scale vortex structures and instead accumulating in strain-dominated regions.

At $\mathrm{St}_k = 0.125$, the strongest negative correlation (-0.1942) is observed, implying that low-inertia particles remain most influenced by vortical flow structures. As St_k increases, the correlation magnitude systematically weakens, reaching its lowest value at $\mathrm{St}_k = 8$ (-0.1144). This progression suggests that as inertia increases, particle clustering becomes less dependent on small-scale turbulence and more influenced by large-scale strain dynamics.

These findings align with previous studies on preferential concentration, reinforcing that low-to-moderate St_k particles exhibit the strongest clustering behavior, while high-St_k particles transition to a more uniform spatial distribution. Furthermore, the weak correlation values indicate that while the Q-criterion provides insight into vortex-particle interactions, other flow characteristics such as strain rate or energy dissipation rate may serve as stronger indicators of preferential concentration at higher St_k values.

Overall, this study highlights the intricate interplay between particle inertia and turbulent structures, demonstrating that clustering mechanisms evolve with increasing St_k. The observed trends suggest that while vortex avoidance remains a fundamental characteristic, the dominant factors governing preferential concentration shift with varying inertia, necessitating further exploration of alternative turbulence metrics to fully capture these dynamics.

VII. Conclusion

This study provides insights into the effects of particle density on preferential concentration and clustering in turbulent flows. By maintaining a fixed Stokes number of unity and varying the fluid-to-particle density ratio, the simulations revealed a nuanced relationship between particle density and turbulence structures. The analysis confirmed that higher density ratios enhance clustering intensity, as shown by elevated RDF values and pronounced particle aggregation in strain-dominated regions. The exception observed at $\rho_p = 300$ highlights the influence of intermediate densities, where transient turbulence-particle interactions may dampen clustering effectiveness.

The peak clustering observed at $\rho_p = 500$ indicates an optimal balance of inertia and fluid coupling for this density, while higher densities $(\rho_p = 800 \, \text{and} \, 1000)$ sustain strong clustering without surpassing the peak. These findings underscore the dominant role of the Stokes number in determining clustering behavior, with particle density acting as a critical modulator of interaction intensity with turbulent flow structures.

Overall, this work contributes to a deeper understanding of particle-laden turbulence by clarifying how density influences preferential concentration and clustering patterns. These insights have practical implications for applications such as pollutant dispersion, aerosol dynamics, and chemical reactor design. Future research could explore higher Reynolds numbers, variable Stokes numbers, and additional forces such as gravity to further uncover the mechanisms underlying particle-turbulence interactions.

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