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Simulation Study on the Mixing Process of Polydimethylsiloxane/Carbon Fiber Composites

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Abstract

Uniform filler dispersion is vital to form thermal networks within polymer composites. Planetary centrifugal blending enables high-quality composite fabrication, yet the microscale dispersion mechanism of carbon fiber (CF) in polydimethylsiloxane (PDMS) remains unclear. This work adopted EDEM-based discrete element simulation to explore the dispersion characteristics of CFs in PDMS during planetary centrifugal stirring. With mixing deviation as the quantitative evaluation indicator, the effects of CF loading, mixing time and mixing speed on dispersion uniformity were analyzed. The results showed that increasing CF content within 1-5 vol% improved dispersion uniformity by strengthening inter-fiber collisions and breaking agglomerates. Optimized processing parameters (6-12 min mixing time and 600-1200 rpm mixing speed) effectively enhanced fluid shear and particle movement to homogenize CF distribution. However, excessively long stirring duration and excessive mixing speed generated parallel particle flow trajectories and suppressed valid inter-particle collisions. Specifically, a high mixing speed of 1400 rpm induced prominent fiber orientation and slight secondary re-agglomeration, thereby degrading the mixing quality. The multi-scale coupling analysis of macroscopic statistical data and microscopic flow field evolution clarified the intrinsic particle-scale dispersion mechanism of PDMS/CF composites.

Keywords: *PDMS/CF composite; Homogeneous mixture; EDEM; Mixing speed; Mixing time*

1 Introduction

With the rapid miniaturization and high-power integration of modern electronic devices, efficient thermal dissipation has become a critical bottleneck restricting device stability and service life[1,2]. Benefiting from low density, good flexibility, superior corrosion resistance and facile processability, polymers have been widely applied in electronic packaging and industrial thermal management [3]. Nevertheless, the intrinsically low thermal conductivity [often $\leqslant$ 0.5 W/(mK)[1]] greatly limits their practical application in high-efficiency heat dissipation scenarios. Embedding thermal fillers into polymer matrices has become a mainstream and effective strategy to fabricate thermally conductive composites[4,5].

The thermal performance of polymer composites significantly depends on the integrity and continuity of filler networks, where uniform filler dispersion is an essential prerequisite. Duing blending processes, microscale fillers easily aggregate under van der Waals forces and electrostatic adsorption[6]. Severe filler agglomeration disrupts the continuity of filler network, and ultimately degrades the thermal performance of polymer composites. The dispersion quality is governed by the dynamic competition between inter-filler agglomeration forces and external flow shear force. Compared with the inherent filler agglomeration characteristics, the shear-induced dispersion effect can be effectively tailored by optimizing mixing techniques and processing parameters. As an advanced manufacturing method, planetary centrifugal mixing integrates chamber revolution and autorotation to generate complex flow gradients and strong centrifugal-shear coupling effects. This unique working principle effectively breaks filler agglomerates and improves filler uniformity, exhibiting distinct advantages over conventional stirring methods. Although this technique has been widely adopted to

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prepare mixtures, most available studies only focus on the macroscopic relationship between processing parameters and thermal performance of mixtures. The microscale dynamic dispersion behavior of fillers during planetary centrifugal blending, as well as the underlying particle-level dispersion mechanism, remains insufficiently clarified, restricting the precise optimization of this blending process[7,8].

In this study, polydimethylsiloxane (PDMS) was selected as polymer matrix and carbon fiber (CF) served as thermal filler. Based on EDEM software[9], the dispersion evolution of fillers varying with filler content, mixing time and mixing speeds was studied. By correlating macroscopic mixing deviation statistics with microscopic particle flow field characteristics, this study aims to reveal the intrinsic dispersion mechanism of PDMS/CF composites, providing theoretical support and process guidance for the fabrication of polymer composites.

2 Simulation Experiments

2.1 Model construction

Planetary centrifugal vacuum mixers realize homogeneous mixture blending through the coupled revolution and autorotation of the mixing chamber. The dual rotational motions (revolution and autorotation) impose strong centrifugal loading to drive intense relative particle movement inside the cavity. A cylindrical mixing chamber with an inner diameter of 60 mm and axial length of 47 mm was established within the EDEM simulation framework [Figure 1(a)]. Identical clockwise rotational velocity was prescribed for both chamber revolution and autorotation. Particle dimensions were reasonably scaled to accelerate simulation computation: PDMS was represented by 0.55 mm spherical discrete elements, while CF was modeled as cylindrical particles with a 0.055 mm cross-sectional diameter and 6 mm fiber length. All particles were initialized via static generation, with a preset settling velocity of 1 mm/s. The particle injection rate was defined as 500 particles/s for PDMS spheres and 100 particles/s for CF cylinders. After bulk particle filling finished, the mixing simulation commenced, with gravitational acceleration (9.81 m/s^2) adopted as the sole external environmental field. Polyvinyl chloride (PVC) was assigned as the chamber wall structural material. Key intrinsic material parameters are summarized in Table 1. For contact mechanics assignment, the Johnson–Kendall–Roberts (JKR) adhesion model was applied for PDMS–CF inter-particle contacts, PDMS self-contacts, and PDMS–PVC wall interactions. The standard Hertz–Mindlin (no slip) contact model was deployed for CF inter-particle collisions and contact between CF segments and the chamber inner wall.

Table 1 Material physical parameters adopted in EDEM simulations

Materials	Density (kg/m^3)	Shear Modulus (Pa)	Poisson's Ratio
PDMS	1030	1.715×106	0.49
CF	2200	6×1010	0.25
PVC	1450	3.501×109	0.30

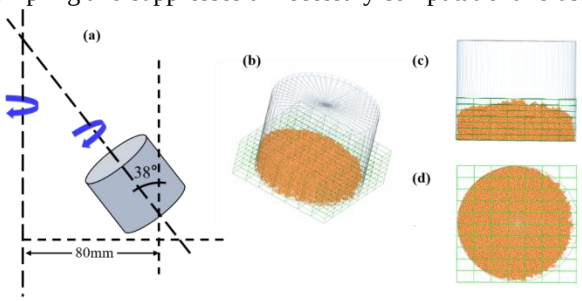
2.2 Evaluation metric for particle mixing uniformity

Mixing deviation (σ) was adopted as the quantitative indicator to characterize filler dispersion quality. With the built-in meshing module embedded in EDEM, the mixing chamber computational domain was discretized uniformly along the X, Y and Z axes to generate a total of n^3 cubic voxels [Figures 1(b-d)]. After tallying the particle category and particle count confined within each individual voxel, the local mixing degree of every grid cell alongside the bulk-averaged mixing degree across all voxels can be acquired. σ is subsequently solved via Equation :

$$\sigma = \sqrt{\frac{\sum_{i=1}^{n^3}\left(M_i - \bar{M}\right)^2}{n^3}}$$

where M_i denotes the mixing degree of the *i*-th voxel, and $\bar{M}$ is the average mixing degrees of all voxels.

Referring to the grid layout visualized in Figures 1(b)–(d), the mixing vessel is split into 343 discrete voxels (7 partitions along each coordinate axis). Grid cells holding under 20 particles are eliminated from subsequent statistical calculation, which mitigates measurement noise stemming from inadequate particle sampling and suppresses unnecessary computational bias.



Figures 1 (a) Schematic diagram of the mixing chamber; (b-d) Grid division diagrams.

3 Results and Discussion

3.1 Effect of filler content

Figure 2 shows the effect of CF contents on the mixing deviation. Obviously, mixing deviation shows a clear monotonic reduction as CF loading increases under identical stirring operating conditions. A peak value of 0.56 was obtained at 1 vol% CF. Progressive declines in mixing deviation were recorded with the increasing of filler loading, with approximate values of 0.55, 0.53, 0.49 and 0.478 for CF of 2, 3, 4 and 5 vol%, respectively. Such a downward tendency stems from amplified inter-filler collision behaviors at higher CF loading level during planetary centrifugal blending. Greater contact frequency between individual CFs breaks filler agglomerates subjected to centrifugal shear stress, restraining cluster regeneration and improving bulk dispersion performance. The results indicate that raising CF content within the 1-5 vol% range promotes the uniform dispersion of filler, which provides desirable microstructural prerequisites to construct interconnected filler networks in the samples.

3.2 Effect of mixing time and mixing speed

As for the mixing time [Figure 3(a)], mixing deviation decreases sharply from 6 to 12 min, after which the curve plateaus with negligible variation at 14 min; this indicates that prolonged stirring beyond the equilibrium durations brings negligible improvement in filler dispersion. Figure 3(b) shows the variation of mixing deviation under different mixing speeds. It is obvious that mixing deviation decreases persistently with the mixing speed increase from 600 to 1200 rpm, indicating more uniform filler distribution. However, 1400 rpm triggers a slight growth of deviation, meaning excessive mixing speed weakens filler dispersion quality.

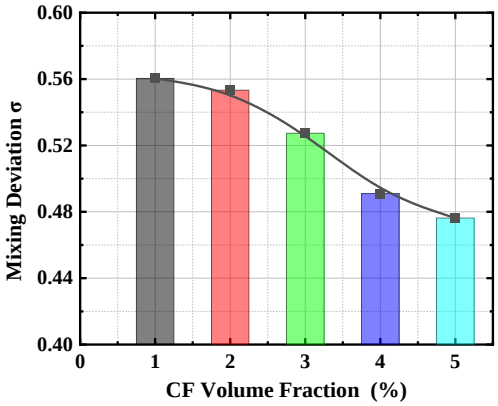


Figure 2 Mixing deviation varying with CF loading level

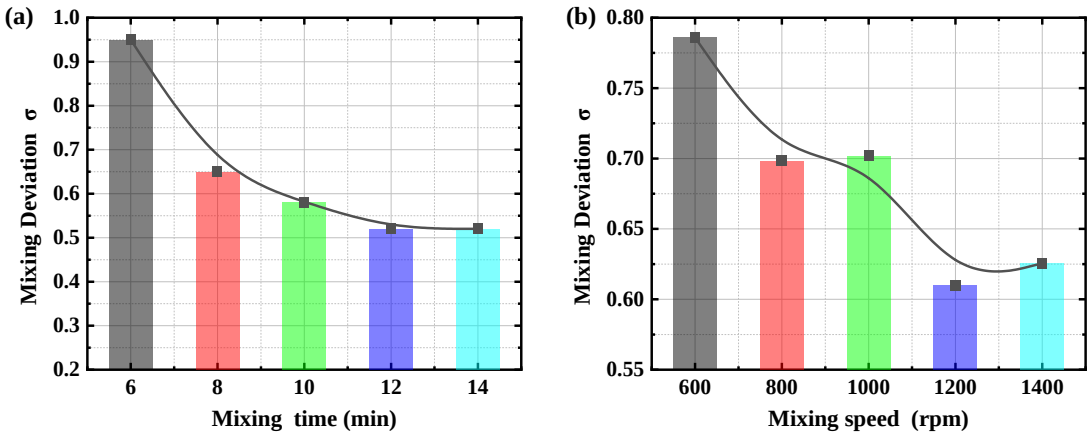


Figure 3 Evolutions of mixing deviation varying with: (a) mixing time, and (b) mixing speed

The microscale particle kinematic features captured by velocity nephograms (Figure 4 and 5) elaborate the underlying physical mechanisms governing the above macroscopic pheonomenon (Figure 3). As for mixing-time (Figure 4), at the mixing duration of 6 min, distinct discrepancies exist in the flow orientations of particles. The resulting relative velocity drives frequent inter-particle collisions, which continuously break CF agglomerates under shear loading and improve filler dispersion, corresponding to the sharp decline of macroscopic mixing deviation. When mixing lasts for 12 min, the flow trajectories of most particles become nearly parallel with negligible relative velocity, bringing inter-particle collisions to a near halt so that the dispersion enhancement relying on collision-induced cluster fracture no longer works. Further extending the mixing duration to 14 min produces no noticeable shifts in particle velocity magnitude and flow orientation, as the spatial arrangement of fillers reaches dynamic equilibrium. Extra stirring time fails to further upgrade dispersion homogeneity, which explains the stable plateau segment observed on the mixing deviation curve with negligible process optimization benefits.

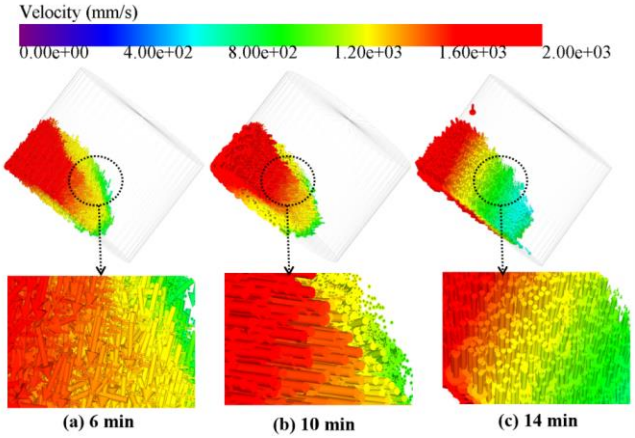


Figure 4 Particle velocity contour distributions at mixing time of: (a) 6 min; (b) 10 min; (c) 14 min

For the mixing speed (Figure 5), as mixing speeds below 1000 rpm, prominent differences in particle flow directions create considerable relative velocity, triggering frequent inter-filler collisions during mixing. Sustained collision and shear effects continuously disintegrate filler agglomerates, thus steadily improving CF homogeneity and reducing mixing deviation. When the mixing speed rises to 1400 rpm, nearly parallel particle flow trajectories are observed with negligible relative velocity, which greatly suppresses inter-particle collisions and invalidates the cluster-breaking mechanism dominated by particle impact. Further increasing the mixing speed cannot promote the uniformity of filler spatial distribution; severe fiber orientation induced by excessive centrifugal force even may cause slight secondary re-agglomeration, leading to a mild rebound of macroscopic mixing deviation.

Combined the results of mixing deviation statistics and particle flow fields demonstrates that moderate mixing time and mixing speed facilitate uniform filler dispersion. Excessively harsh mixing parameters weaken dispersion performance; the revealed particle-level mechanisms provide guidance for optimizing the preparation process of PDMS/CF composites.

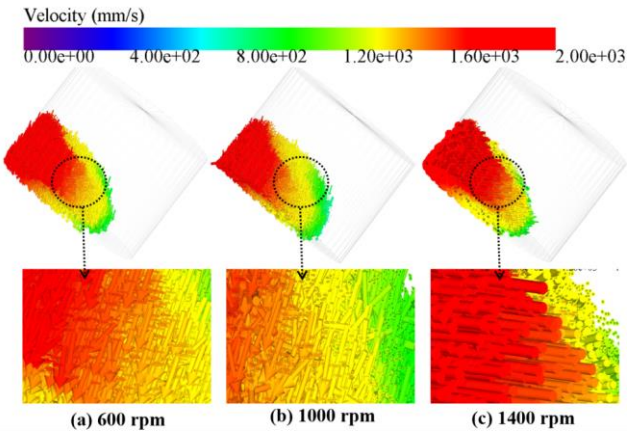


Figure 5 Particle velocity contour distributions varying with mixing speed: (a) 600 rpm; (b) 1000 rpm; (c) 1400 rpm

4 Conclusions

In this study, discrete element simulations based on the EDEM software were performed to investigate the dispersion behavior of CFs within PDMS matrix by planetary centrifugal blending, where mixing deviation was adopted as the quantitative index to evaluate filler homogeneity. The effect of three parameters (namely CF fraction, mixing time and mixing speed) on the the dispersion quality of PDMS/CF composites were studied. Within CF loading level of 1-5 vol%, elevated filler concentration effectively reduced mixing deviation and promoted uniform CF distribution, which was attributed to intensified inter-filler collisions that disintegrate fiber agglomerates. Enhancing mixing time from 6 to 10 min, and mixing speed from 600 to 1000 rpm also facilitated filler homogenization via enhancing fluid shear and particle contact frequency. However, obvious performance plateaus emerged once mixing time exceeded 12 min and mixing speed surpassed 1200 rpm; further increasing either parameter generated negligible improvements in dispersion uniformity, while a mixing

speed of 1400 rpm even degraded mixing performance. These findings deliver clear theoretical guidance and process optimization references for the fabrication of polymer composites via planetary centrifugal blending, and offer generalizable insights for the formulation design of other polymer composites.

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References

[1] He, X., Li, Q., Li, L., et al. Preparation of a flexible polymer-based phase change composite with enhanced thermal management enabled by low-heat-dissipation structure [J]. Thermal Science and Engineering Progress, 2026, 69: 104433.

[2] Wu, J., Yang, T., Wang, K., et al. Revealing the role of molecular weight on mechanical reinforcement of highly oriented UHMW-PE fibers [J]. Polymer, 2025, 317: 127953.

[3] He, L., Dou, Z., Zhang, Y., et al. Modelling Effective Thermal Conductivity in Polymer Composites: A Simple Cubic Structure Approach [J]. Composites Science and Technology, 2020, 184: 107775.

[4] Zheng, S., Wang, Y., Guo, L., et al. Research progress of thermally conductive polymer composites with three-dimensional interconnected network structures [J]. Acta Materiae Compositae Sinica, 2023, 40(12): 6528-6544.

[5] Tang, S., Liu, S. L., Cong, B. H., et al. Graph attention networks decode conductive network mechanism and accelerate design of polymer nanocomposites [J]. NPJ Computational Materials, 2025, 11: 280.

[6] Cheremisinoff, Nicholas P. Polymer mixing and extrusion technology [M]. N. Y.: Dekker, 1987.

[7] Kwon Joong Son. Numerical analysis of viscous polymer resin mixing processes in high-speed blade-free planetary blender using smoothed particle hydrodynamics[J]. Processes, 2023, 11(9): 2555.

[8] Xin, Y., Zhu, X., Wang, T.. Mixing characteristics of polymer melt in triple screw extruders with combined screws using finite element method[J]. IOP Conference Series: Materials Science and Engineering, 2020, 768(2): 022068.

[9] Graziano Frungieri, Gianluca Boccardo, Antonio Buffo, et al. CFD-DEM characterization and population balance modelling of a dispersive mixing process[J]. Chemical Engineering Science, 2022, 260: 117859.