Generalized Formula of the Fraction of Interphase for Polydisperse Non-Spherical Particles: Theoretical and Numerical Models

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Abstract: The volume fraction of interphase is an important microstructure parameter in the prediction of macroscopic properties of particulate composites. Currently, some researchers have presented theoretical and numerical investigations on the interphase fraction for spherical particle systems, and even quantify the influence of interphase fraction on the overall elastic and transport properties of particulate composites. However, the overlapping interphase fraction in polydisperse non-spherical particle systems is still an open issue. In this study, a generic theoretical model is formulated to derive the overlapping interphase fraction for polydisperse 2D non-circular and 3D non-spherical particle systems by means of the statistical geometry of composites. On the other hand, numerical simulations for the one-point probability function of interphase are presented to verify the proposed theoretical framework. In the numerical simulations, a novel algorithm is developed by reducing the problem of identifying the precise location between an arbitrary spatial point and interphase to the basic issue of finding the distance from the point to the surface of particles. If the distance is less than the interphase thickness, the point definitely locates inside interphase. In addition, the algorithm can be further used to detect the overlap between adjacent ellipsoidal particles (2D ellipses). Moreover, a variety of particle shapes (such as regular polygons and ellipses with the same circularity, and regular polyhedrons and ellipsoids with the same sphericity) are taken into account to generate particle packing structures. Then, the fraction of overlapping interphase in each packing structure is statistically obtained. Results show that statistical values are consistent with their theoretical values under the same conditions. This validates the reliability of the theoretical framework.

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