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Detailed Simulation of Particle and Liquid Distribution in the Mixing Zone of a Twin-Screw Granulator

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Abstract Text: Wet granulation for continuous manufacturing in the pharmaceutical industry can be achieved using a twin-screw granulator, which is emerging as a promising technology. This is due to the high degree of flexibility through varying (i) the screw configuration which has a modular structure and (ii) the process parameters, allowing to achieve mixing and granulation in a short time (in the order of seconds). However, to optimally take advantage of this flexibility, a thorough understanding of the mixing and flow characteristics, which drive the wet granulation in the twin-screw granulator is necessary. Despite the progress that has been made by experimental and meso-scale modelling studies in recent years, the description of the flow and mixing of the wet particulate materials in the twin-screw granulator is still challenging. In this study, we examined the time evolution of the spatial liquid distribution in the kneading section of a twin-screw wet granulation process. Particle scale, discrete element method (DEM) based simulations of a short quasi-two-dimensional simulation domain were performed. A capillary force model, as well a liquid transfer model (Mohan et al., Powder Technol 264: 377–395) were used to account for pendular liquid bridge formation, rupture and inter-particular forces. The analysis of liquid distribution between particles and liquid bridges showed that, if the liquid addition rate and source area are changed, and despite the fact that the same amount of liquid was added to the particles, the partitioning between the liquid present on the particle surface and the liquid bridges changes. For a larger spatial extent of the region in which liquid was added to the simulation, the number of liquid bridges increased. However, again the partitioning of the liquid in the bridges and on the particle surface changed. This suggests a higher aggregation level due to a higher number of liquid bridges, but also the possibility of increased breakage rates in case of high shear treatment due to the weak liquid bridge forces. Our results help identifying key parameters that impact liquid spreading (i.e., solid-liquid mixing) during particle processing in twin-screw granulators. Consequently, our results are an important guide in the future development of advanced closures for mesoscopic models, e.g., population balance models used in industrial applications.

Session Selection:
Particle Engineering as Applied to Pharmaceutical Formulations
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Detailed Simulation of Particle and Liquid Distribution in the Mixing Zone of a Twin-Screw Granulator
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Pharmaceutical Engineering and Drug Delivery

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