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Electrostatic effects in granular media

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Electrostatic charging via contact electrification or tribocharging refers to the process of charging of two solid surfaces when they are brought into contact and separated. In pharmaceutical formulation processes, particle charging is often a nuisance and can cause problems in the manufacture of products, such as powder flow, fill level and dose uniformity. For a fundamental understanding of powder triboelectrification, it is essential to study charge transfer under well-defined conditions. Hence, all experiments in the current study were separately conducted in a Hopper-Chute Assembly and a V-blender located inside a glove box with a controlled humidity of 20%. To quantify the electrification of powders, different contact surfaces viz. PVC, aluminium, Teflon, PMMA were employed along with 2 pharmaceutical excipients and 2 drug substances. Tribocharging of drug-excipient mixtures was attempted via a blending process. Moreover, the collisional nature of triboelectrification was investigated using a 3D DEM model incorporating charge transfer and electrostatic forces. For the pharmaceutical materials, the chemical potential was calculated using MOPAC, a semi-empirical molecular orbital package which has been previously employed for the solid state studies and molecular structure predictions. Based on the chemical potential values, a triboelectric series of pharmaceutical materials was generated, which seems to suggest that electrons are the charge transfer agents. Bipolar charging is a special case of triboelectrification observed between the surfaces of the same material, acquiring opposite polarities based on particle size differences. The intricacies and complications of the polarity induced by bipolar charging is often suppressed by the dominant particle wall interactions in the premise of the net final charge of the system, undermining the charge mitigation approaches in process manufacturing and incapacitating the complete alleviation of its enmeshed disadvantages. Surface characterization for two different sizes of lactose and MCC were done by multiple analytical techniques including, X-ray photoelectron spectroscopy, energy dispersive X-ray spectroscopy, interferometer-profilometer studies, scanning electron microscopy, dynamic vapour sorption studies and thermo-gravimetric analysis. Analytical methods confirmed the differences in surface roughness, surface impurity and surface moisture contents between different particle sizes of the same material. The MCC particles showed differences in moisture content at different RH conditions; however the same was not evident in lactose monohydrate. The effects of bi-polarity in similar materials were further studied with glass beads in a specialized assembly made up of glass, using the concept of Brazil nut effect to segregate particles based on size differences under controlled vibration. The trends obtained from the collected samples indicated differences in polarity between two different sized glass beads. A multi-scale model was developed using quantum (DFT) models and bulk-scale (DEM) models to study the electrostatics behaviour in the granular media. The computational model validated the magnitude of frequency and amplitude implemented to obtain the Brazil nut effect for the specialized assembly in the experimental set up and confirmed specific regimes of segregation and mixing, observed during the experiments. Depending on the moisture content per unit surface area, particle of the same material was found to acquire positive or negative charges during contact electrification. The charge profiles of lactose, MCC and the glass beads obtained from DEM calculations were similar to the experiments and followed the work function differentials obtained from DFT and semi-empirical calculations.

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