

The use of Discrete Element Method (DEM) modelling to study the de-agglomeration of pharmaceutical dry powders for inhalation

**M.S. Coates¹, D.F. Fletcher¹, H-K Chan¹, J.A. Raper¹, R.Y. Yang²
and A.B. Yu²*

¹ University of Sydney, Sydney, Australia

² University of New South Wales, Sydney, Australia

For many years Respiratory Drug Delivery has been recognized as a desirable route for drug delivery to the body and has attracted a large amount of research activity. In order to achieve a correct and reproducible delivered dose, a rigorous understanding of how the powder agglomerates interact with air-flow to de-agglomerate and disperse is required.

The de-agglomeration of drug particles to form a fine respirable aerosol cloud is thought to be achieved by three major mechanisms: 1) Particle interaction with shear flow turbulence, 2) Particle-device impaction, and 3) Particle-particle impaction. The aim of this study is to isolate each de-agglomeration mechanism and to determine its relative effect on overall powder de-agglomeration.

This study uses Discrete Element Method (DEM) modelling to study the nature of the break-up of randomly formed agglomerates by de-agglomeration mechanisms two and three. Studies of particle-wall impactions and particle-particle impactions were performed for a variety of initial velocities and impact angles. These data were then used to construct simple correlations that can be fed back into CFD simulations of the flow within dry powder inhalers to predict fine particle generation.