# EPSRC supported EngD Predicting pharmaceutical manufacturability using multiscale DEM

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**Tax free bursary of £25,000 p.a. plus fees paid**

In the early development of new active pharmaceutical ingredients (APIs), pharmaceutical scientists often have access to only small amounts of material for testing. Even as we move through the development and commercialisation process, the reduction in the amount of API used for experimental purposes will significantly reduce a project’s carbon footprint. As such, the ability better characterise, and thus predict the behaviour of, new APIs can not only help accelerate the development of new products, but also reduce waste and thus improve the sustainability of this development.

This project will utilise Discrete Element Modelling (DEM) simulation to comprehensively understand how fundamental particle properties define APIs’ bulk behaviours. The successful applicant will conduct virtual tests on particles with diverse fundamental properties, exploring e.g. packing, compressibility, permeability, cohesion, coordination number, and shear strength. Based on the DEM simulations, AI models will be implemented to allow the prediction of these mesoscale properties. The AI model's predictions will serve two primary purposes: i) establishing further correlations with relevant bulk properties of actual materials, thereby bridging fundamental properties with macroscopic behaviour, and ii) laying the groundwork for a multiscale modelling framework applicable to simulations of real equipment such as feeders, blenders, or tablet presses.

To be eligible for EPSRC funding candidates must have at least a 2(1) in an Engineering or Scientific discipline or a 2(2) plus MSc. To apply please email your cv to cdt-formulation@contacts.bham.ac.uk. Currently, we are only able to accept UK nationals. For details on the Engineering Doctorate scheme visit the homepage.

Deadline: 26th July 2024