Virtual prototyping of particulate processes – Design and optimisation of the wet granulation process via multiscale modelling & rapid prototyping

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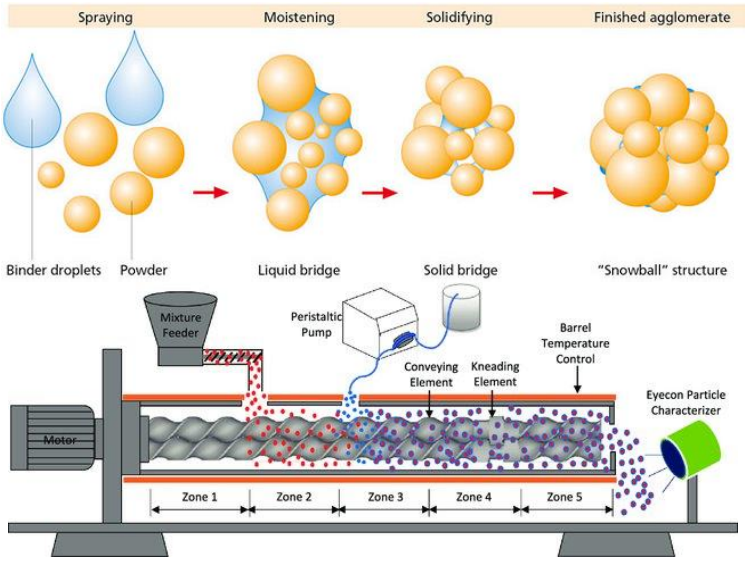
Wet granulation produces enlarged granules with a homogeneous size distribution from a mixture of particulates and liquid binder. It is a key process in the pharma, agro-chemical and food industries to improve the flowability of powders and to mix materials that would otherwise cake (agglomerate) or segregate. Industry is now aspiring to move from batch operations (rotating drums, tumblers) towards continuous processes (twin-screw, fluidised bed, extrusion) to increase output, provide consistent quality, and reduce operator involvement [1]. A PhD project is currently underway to address this need, applying multiscale modelling tools to the continuous twin-screw granulator, see Figure [1], which has the added advantage of mixing the particulates under high shear. To date, no comprehensive model exists to predict this process, and the screw has to be empirically adjusted to achieve a homogeneous size distribution [2]. A computer model that can predict the dispersion and growth of the particle size in terms of screw shape, particle and fluid properties will shorten the optimisation effort, and lead to more efficient screw designs by virtual prototyping of the process.

There are many possibilities for a student project to make a contribution, for example on the following topics:

1. Develop a **3D printable model** of a twin-screw granulator, which will be used for validation and calibration purposes. 3D printing offers easy customisation, allowing us to quickly test different designs and to explore the scalability of the process.
2. Take experimental data on a real wet-granulation process at one of our i**ndustrial project partners**.
3. Develop part of the **numerical model**. We aim to develop a multiscale approach to simulate the wet granulation process, coupling discrete particle simulations (DEM) on the microscale with a continuum flow model (FVM-PBM) on the bulk-scale. Many parts of this model still have to be determined and you can be part of the development team. The code will be open-source, as part of MercuryDPM.org, so a successful code development will gain you recognition in the academic community.
4. Learn how to calibrate numerical models. We use a novel and advanced **machine-learning algorithm (GrainLearning)** to calibrate micro-scale parameters from experimental bulk measurements. Apply this algorithm, and gain experience in the rapidly developing field of machine-learning.



Top: Illustration of the wet granulation process [3], bottom: Schematic of twin screw granulation [4].

References:
[1] A Kumar *et al*. Eur. J. Pharm. Biopharm., 85(3 PART B):814–832, 2013.
[2] A Eitzlmayr *et al*. Int. J. Pharm., 474(1-2):157–176, 2014.
[3] A Katari. Retrieved from https://doi.org/doi:10.7282/T3R214K8
[4] H Liu *et al*. Computers & Chemical Engineering. 125. 10.1016, 2019.