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Modelling of co-rotating twin-screw extruders in the pharmaceutical industry I: single component model

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Twin-screw extruders are being increasingly applied in the pharmaceutical industry for the manufacture of solid dispersions. In particular, Hot Melt Extrusion (HME) is a viable manufacturing alternative for poorly soluble drugs that are difficult to process. This is due to the high shear stress applied in the process, which enhances mixing of the base polymer with the dispersed API. Delivery systems that can be obtained using this technology include pellets, granules, sustained release tablets and implants. Experiments for HME are typically very labour-intensive, involving the use of highly viscous polymers, high pressures, and require proper cleaning between runs. Identifying the critical experiments to perform based on model simulations would thus be highly desirable. Single-component modelling of twin-screw extrusion processes could be beneficial in the following areas: identifying optimal screw configurations, tracking the degree of melting and when identifying the area within the extruder where the polymer becomes completely melted.

An axially distributed mechanistic model of HME was previously developed by Eitzlmayr et al.[i], wherein the extruder elements were described using physically-meaningful parameters estimated from experimental data and any given extruder could be built into the model in a modular way. Their model was implemented into gPROMS FormulatedProducts[®], and the simulation results obtained for different HME configurations using Soluplus[®] were reproduced. Important process variables such as filling ratio or element pressure, which are often difficult to measure, were given as simulation outputs; measurable variables, including the temperature of the screws and the melt and residence time distribution, were validated against experimental results obtained in a 40:1 ThermoFisher Eurolab co-rotating twin-screw extruder at CMAC. In addition, experiments with a chosen extruder configuration operating under fixed conditions were carried out with Soluplus[®], Plasdone[™] and Affinisol[™]. The effect of polymer nature on screw element parameters (A1, A2 model parameters) was investigated by comparing the results obtained across the three polymers.

Overall, the existing model was proven to perform well for the single component polymer case. Further work focuses on extending this model to account for multi-component mixtures and capturing API solubility.

i. Eitzlmayr, A., Koscher, G., Reynolds, G., Huang, Z., Booth, J., Shering, P. and Khinast, J. (2014) "Mechanistic modeling of modular co-rotating twin-screw extruders", *International Journal of Pharmaceutics*, 474(1), 157-176.