Poster Presentations

[MS39-P01] Applications of Synthonic Engineering tools in predicting crystal morphology as a function of the growth environments

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There is a critical need in industry to get a desired morphology of a crystal in order to have control in downstream processing or flow properties and product yield. All crystalline products produce molecular analogues from side reactions and/or processing. These molecular analogues as additives/impurities and solvents may have an effect on the growth of the crystals leading to different physical and chemical properties which will in turn have an effect on the formulation behaviour. Therefore, the understanding of these crystal growth modifiers and their interactions with the host is critical in manipulating the host system to obtain a morphology that is most suitable for product formulation and processing requirements. VisualHABIT is a molecular modelling tool[1-4] routinely used to understand, predict and manipulate crystal growth morphology but with an added user-friendly graphical user interface. The morphology prediction is on the basis that the surface attachment energy of a particular crystal face is assumed to be proportional its relative growth. The attachment energy is the contribution from all the interactions that are normal to the growth surface (hkl). Thus, a quantitative analysis of the intermolecular forces (synthons) involved in the growth processes is provided by a systematic search approach within VisualHABIT. This knowledge of the strengths and contributions of intrinsic synthons (solute/solute) and extrinsic synthons (solute/solvent or solute/crystal growth modifiers) to the growth process enables the understanding and prediction of the effects of the crystallisation environment on crystal morphology.

This research was carried out as part of an EPSRC follow-on grant and it provides a molecular level understanding of industrial applications through case study examples. These case studies include the effects of different solvents on the morphology of an active pharmaceutical ingredient, solvent effect on the growth morphology of an ester, comparison of the effects of solvents on the growth morphology of hydrates and anhydrates and the effects of solvents on the crystal morphology of benzophenone.

References

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