CryArc Submission: Solubility Curves, Crystal Nucleation and Growth Kinetics of para-Nitrophenol

Jason Neagle[1], Brian Ramirez[1], Lily Rhoads[1], Salatan Duangdangchote[2], Peerapon Rapeenun[1], Gerard Capellades[*1]

[1] *Department of Chemical Engineering, Rowan University, Glassboro, 08028, New Jersey*

[2] *MAPLE INFINITE CORPORATION, 40 Holland Park Ave, York, ON, M6C 1M3, Canada*

Purpose:

A critical bottleneck in crystallization process development is the lack of a curated database for nucleation and growth kinetics paired with high-quality solubility data. CryArc (Crystallization Archive) presents an opportunity for improved predictive crystallization proof of concepts given user entries, validated methodologies and vetted data submissions.

Methods:

Pure para-nitrophenol was prepared for polythermal screening, solvent compatibility and kinetic studies using a Technobis Crystalline. Transmittance and particle detection was used to create solubility curves while also gathering nucleation and crystal growth data for para-nitrophenol in water for parameter estimation. Parameter estimation was completed in gPROMS FormulatedProducts (Siemens Process Systems Engineering) to determine parameters for secondary nucleation and crystal growth.

Results:

Polythermal screening during the heating period will result in decreased transmittance as saturation temperature is approached, providing a value for a proposed solubility curve. The Crystalline allows for particle detection via image analysis during the cooling crystallization of para-nitrophenol, coupled with gPROMS FormulatedProducts, allows for kinetic parameter estimations.

Conclusions:

Once solubility, nucleation and crystallization data are gathered, the workflow using the Crystalline and gPROMS provides an experimentally validated method for parameter estimation. The results from this workflow for para-nitrophenol will be submitted to the public CryArc database, with the included submission containing experimental conditions as well as estimated parameters.

Keywords:

Crystallization, pharmaceuticals, database, modeling, kinetics