



Comparison of One Dimensional and Two-Dimensional Population Balance Model for Optimization of a Crystallization Process

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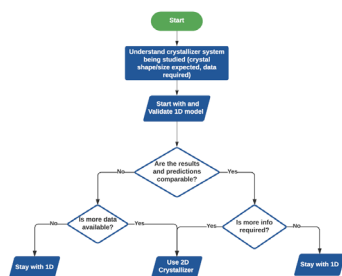
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1. Introduction

- 2D Population Balance Modelling (PBM) offers several advantages to 1D PBMs
- Ability to model two different growth kinetics for the axes, which allows for better predictions for needle or plate-like crystals
- Can account for crystal shape evolution during the crystallization process
- Aim of this work is to develop and validate a 2D PBM model for an API with a plate-like crystal morphology

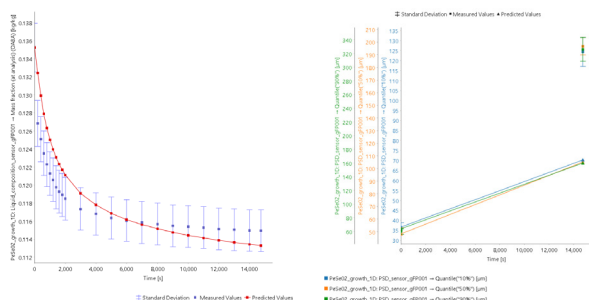
2. Process Workflow



- Workflow summarises the choice of PBM you would use based on the experimental data you have available. In general:
- Start with a 1D PBM model
- If predictions for particle size are poor and the right dataset is available, move onto a 2D PBM model

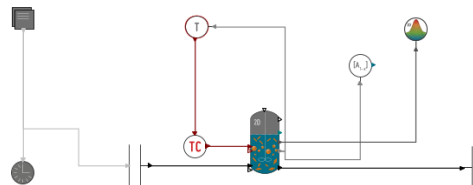
3. 1D Population Balance Model Predictions

- 1D PBM model was developed for the antisolvent crystallization of anthranilic acid and ethanol-water. Lab-scale experimental data was used to validate the model
- The growth kinetics were estimated, and the predicted concentration profile shows a good fit with experimental data.
- The circular equivalent diameter however is significantly underestimated even after several iterations.
- This may be due to the 1D PBM limitations, therefore a 2D PBM model was developed with the 1D kinetic predictions as a starting point for the major axis growth kinetic parameters



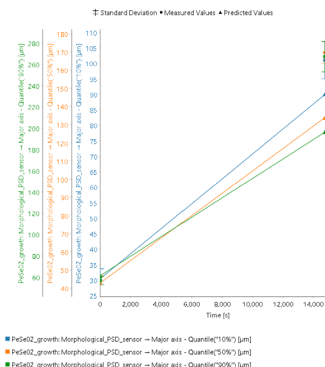
4. 2D Population Balance Model

- The 2D PBM was developed specifically to predict growth kinetics on the major and minor axes.
- Data required to validate the particle size is more detailed than that for the 1D model
- Would require particle size distribution for the major & minor axis and aspect ratio as opposed to a single circular equivalent diameter (laser diffraction)



5. Parameter Estimation

- The 2D PBM predictions showed good agreement for the concentration profile data, which is similar to that seen with the 1D PBM
- More importantly, the predictions for the major axis growth kinetics showed better agreement with experimental data
- The next step would now be to validate the minor axis growth kinetics and optimise the crystallization process



6. Conclusions

- This work shows the workflow for the development of a 2D PBM model for the anti-solvent crystallization of anthranilic acid, which as a plate-like morphology
- The 1D PBM crystallizer model shows good agreement with concentration profile, however it does have poor particle size predictions
- This challenge is addressed by changing the model to a 2D PBM, which allows for the specification of 2 growth kinetics, one for each axis.
- The next step from here is to validate the growth kinetics for the minor axis and optimise the antisolvent crystallization process

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