Application of gCRYSTAL CLD sensor workflow for kinetic parameter estimation

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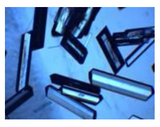
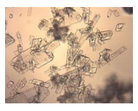
Introduction

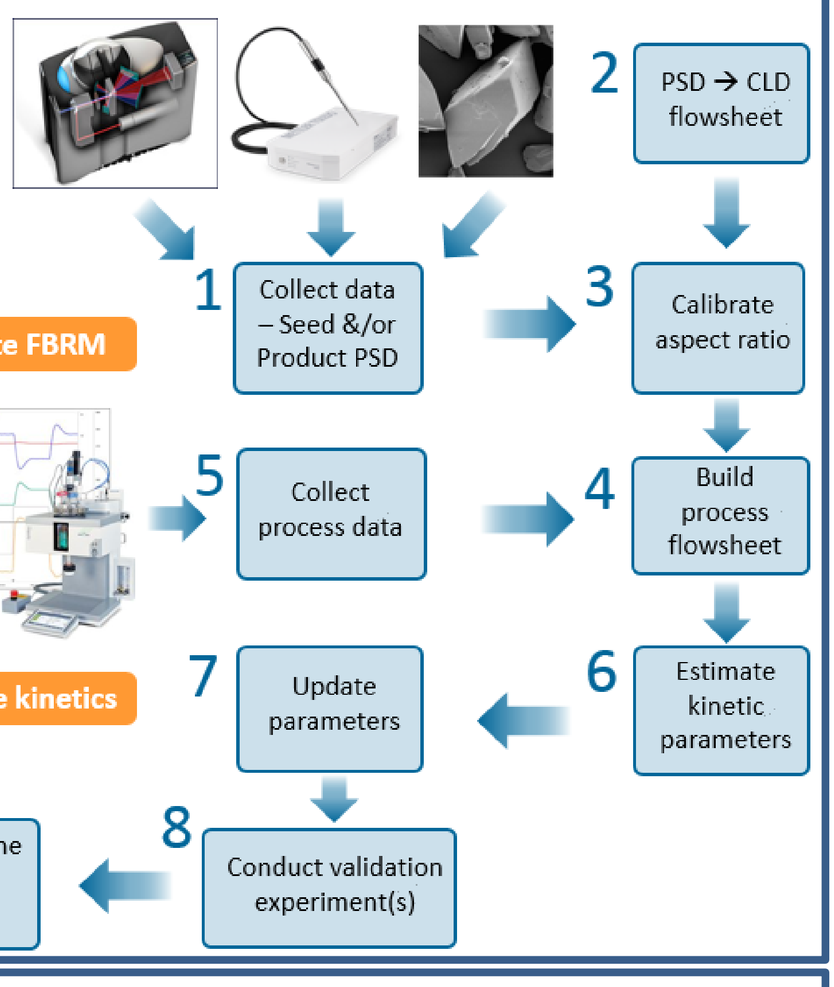




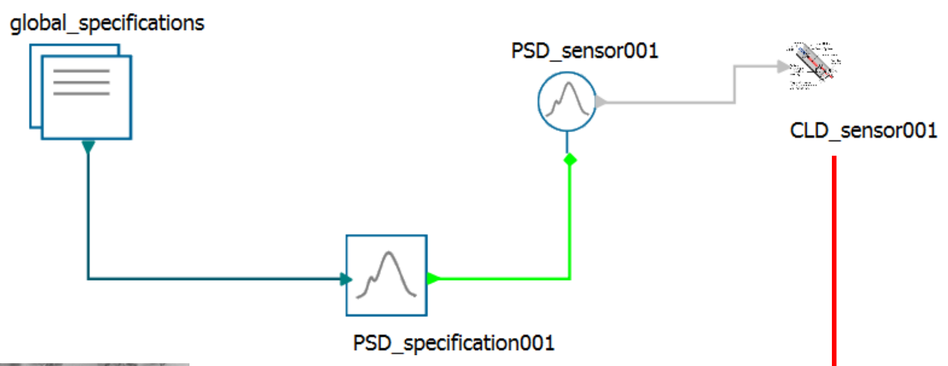
The gCRYSTAL software package contains theoretical models for predicting the particle size distribution (PSD) of particles produced in crystallisation processes. These models contain kinetic parameters whose values need to be tuned for a particular process. This kinetic parameter estimation process may not be successful due to the wide variation in crystallisation process conditions. The estimated kinetic parameter values can be made more accurate by incorporating inline sensor data. The chord length distribution (CLD) data can be used for this purpose.

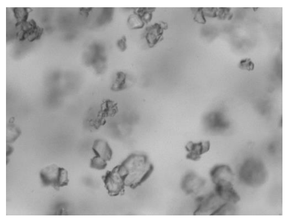
In this joint project between the University of Strathclyde and PSE, we developed a CLD sensor module for the gCRYSTAL package. We also developed a workflow for the application of this CLD sensor module. Here we illustrate the application of this workflow with data collected during a super saturation controlled growth experiment of paracetamol. The experiment was performed at the University of Strathclyde.

Workflow for CLD application in gCRYSTAL for more accurate PSD prediction



Aspect ratio calibration using PSD to CLD forward transformation

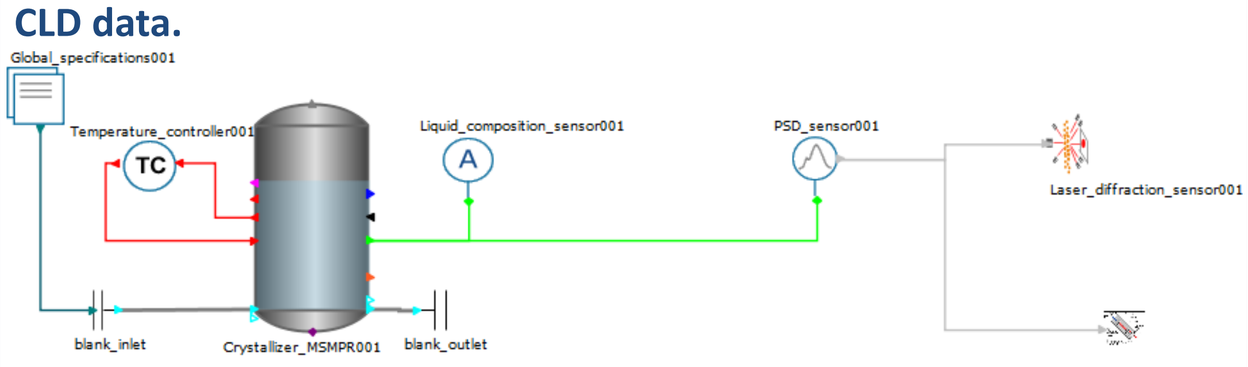




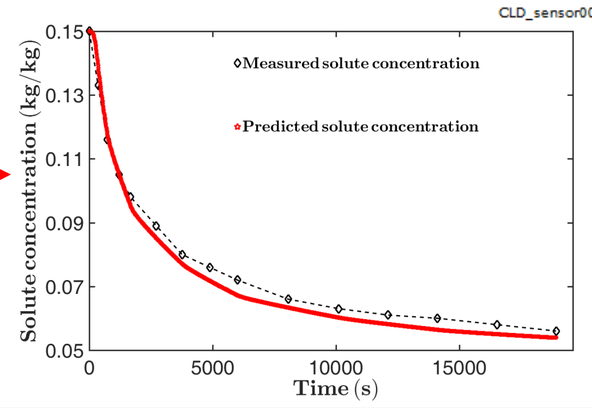
Consistent with shape of particles

Predicted aspect ratio = 0.55

Kinetic parameter estimation using solute concentration, PSD and CLD data.

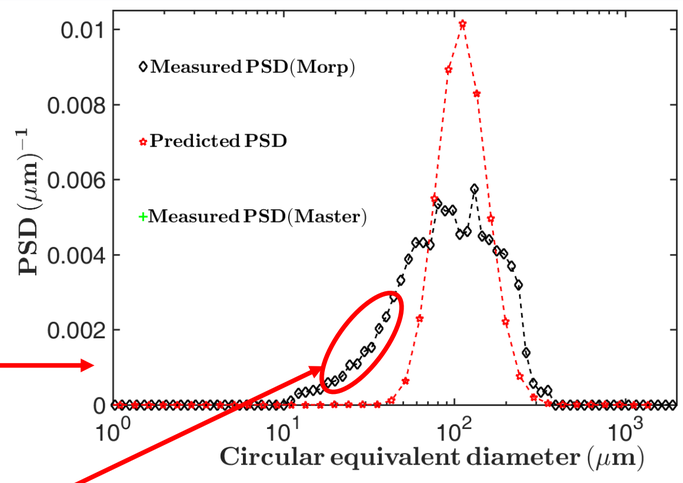


Measured and Predicted solute concentration



PSD prediction

- Measured and Predicted PSD.
- PSD measurement by ofline Malvern Morphologi G3



Discrepancy may be due to breakage and agglomeration associated with offline analysis

	Predicted	Measured
D_{v25} (μm)	99.2	100.5
D_{v50} (μm)	124.4	154.7
D_{v75} (μm)	157.4	220.2

Acknowledgement

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References

*[1] O. S. Agimelen et al., Chemical Engineering Science **123**, 629 (2015).*

*[2] O. S. Agimelen et al., Chemical Engineering Science **144**, 87 (2016).*

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