

A Holistic Approach for the Model-based Control of Crystal Size, Shape and Purity in Integrated Continuous Crystallization – Wet Milling – Classification Systems

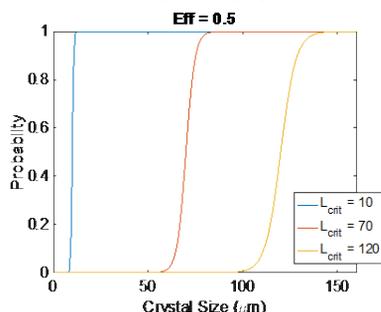
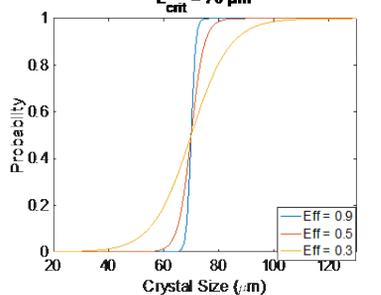
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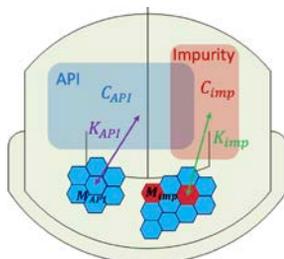
Specific aims: "To develop and provide the first proof-of-concept simulation and experimental demonstration of a real-time implementation of a full population balance model based nonlinear predictive control approach for batch and continuous crystallization processes integrated with wet milling and classification/recycle system, in order to achieve desired crystal size and shape distribution. The effects of impurity/additive mixtures on the size, shape and crystal purity distribution will be incorporated in the model."

Crystallizer – Wet Mill – Classifier

Classification system design ($S = \frac{e^{EX}-1}{e^{EX}+e^{E-2}}$)

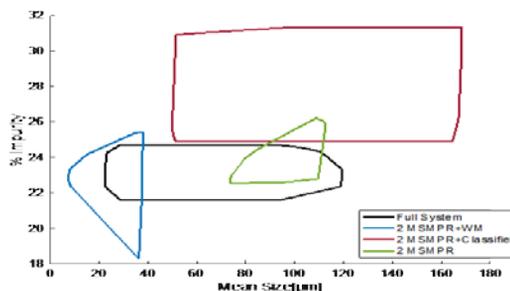


Impurity model development

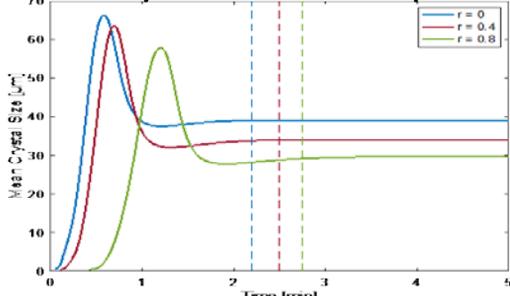


α : partition coefficient
 K : relates solid phase (M) to liquid phase (C)

Attainable region for an integrated system

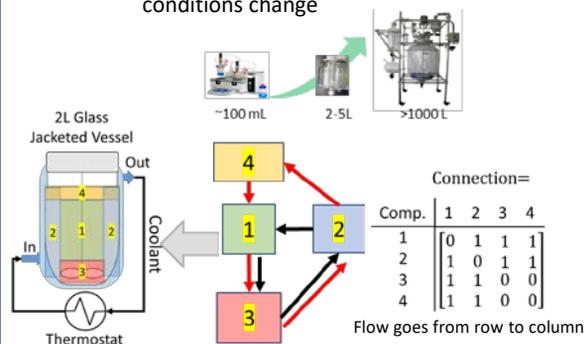


Dynamic model – Startup



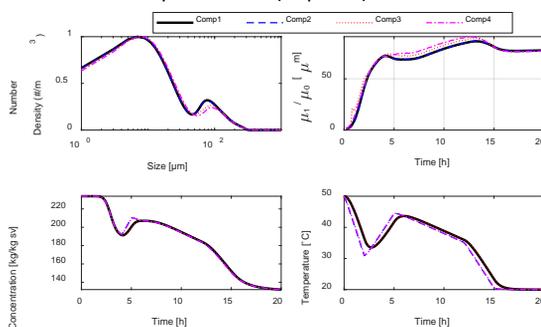
Application – Scale-up

- Batch crystallization scale-up issues:
 - Crystallizer geometry, scale, and operating conditions change



- Unseeded batch thermocycling temperature profile

- Heat transfer delayed in compartment 1 (bulk phase) and compartment 3 (impeller)



Future Plans

- Experimental validation
- Crystallizer network applications
 - Implement flow velocities from CFD simulations
 - Incorporating attrition at impeller
- 2D simulation of the integrated system
- Model based quality by control (Qbc)
 - Developing a moving horizon estimation (MHE) based nonlinear model predictive control using the full 1D and 2D PBMs for size, shape and inferential purity control for both process systems.

