Mathematical modeling, simulation optimization and control of crystallization processes for controlling the particulate properties

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Outline

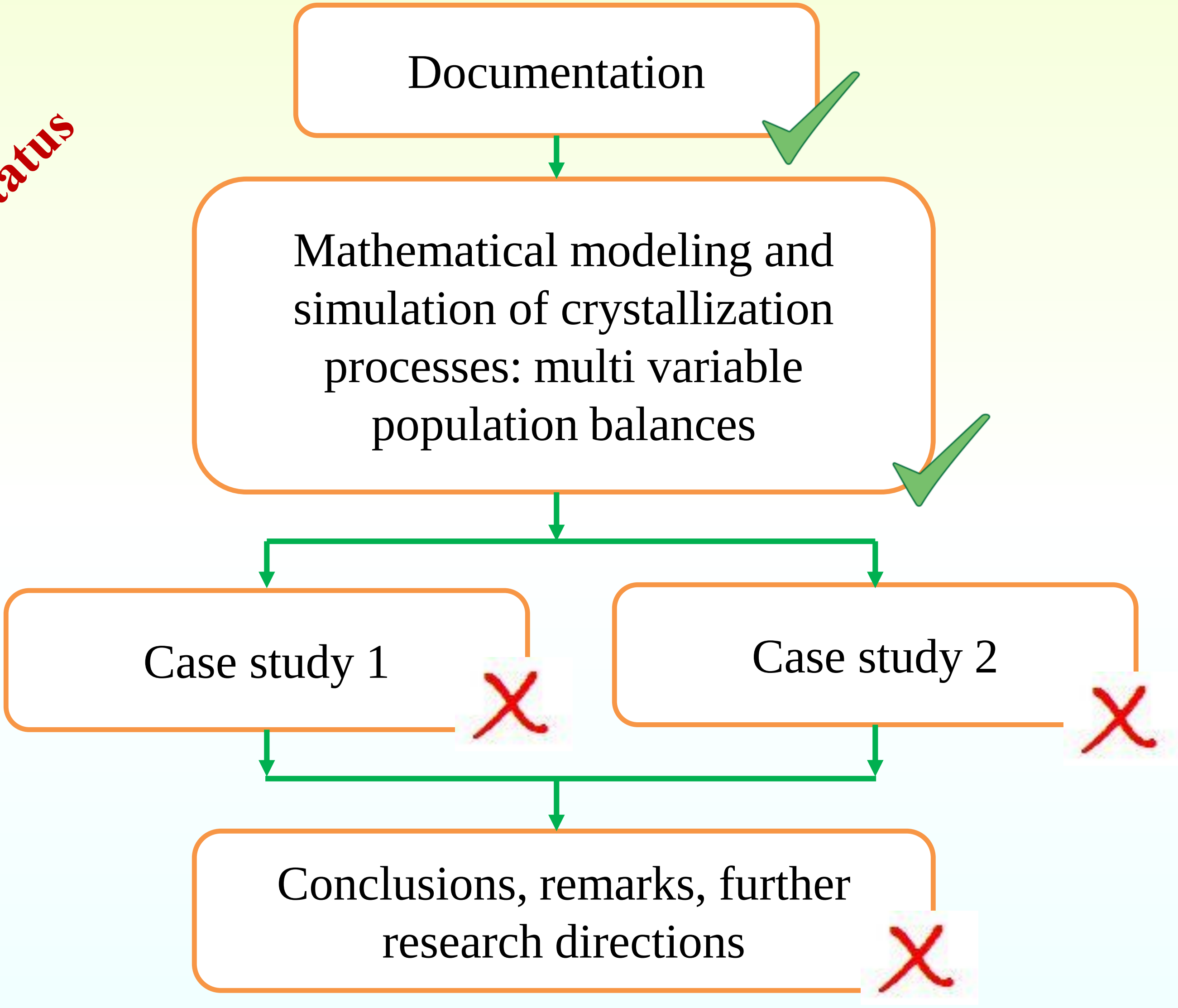
PhD objectives: a short presentation of the main purposes of the thesis

The main results of the first part of PhD summarizing the main results

Future plans
??

PhD objectives

Current status



M-PB: Crystallization of plate-like crystals

- ***Phenomenon of plate-like particle crystallization***

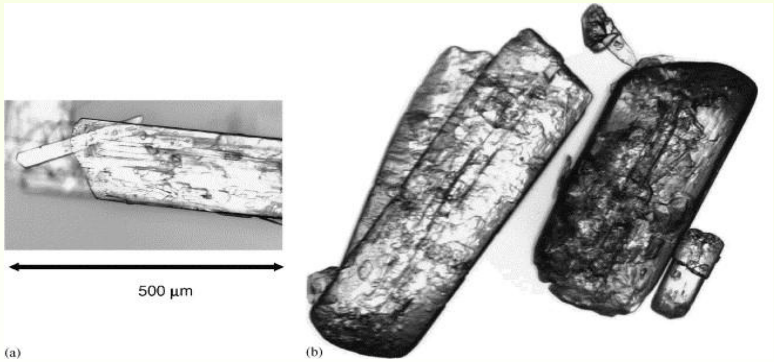


Figure 1. Plate like crystal **[1]**

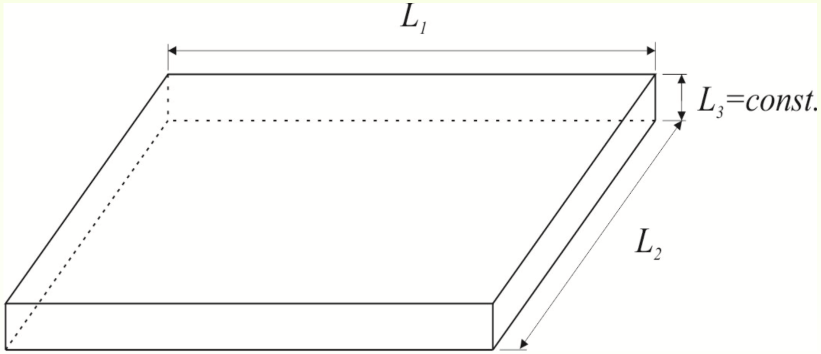


Figure 2. Plate like crystal shape **[2]**

- ***Mathematical model (the population balance only)***

$$\frac{\partial n(L_1,L_2,t)}{\partial t}+\frac{\partial\left[G_1 n(L_1,L_2,t)\right]}{\partial L_1}+\frac{\partial\left[G_2 n(L_1,L_2,t)\right]}{\partial L_2}=B(L_1,L_2,t)$$

With the appropriate initial and boundary conditions

[1] Oullion, M., Puel, F., Fevotte, G., Righini S., Carvin, P., ***Industrial batch crystallization of a plate-like organic product. In situ monitoring and 2D-CSD modelling. Part 1***, Chem. Eng. Sci. 62, 833 – 845 (2007), **[2]** Szilagyi , B., Lakatos, G.B., ***Batch cooling crystallization of plate-like crystals: A simulation study***, Per. Pol. – Chem. Eng, *DOI: 10.3311/PPch.7581*

M-PB: Crystallization of plate-like crystals

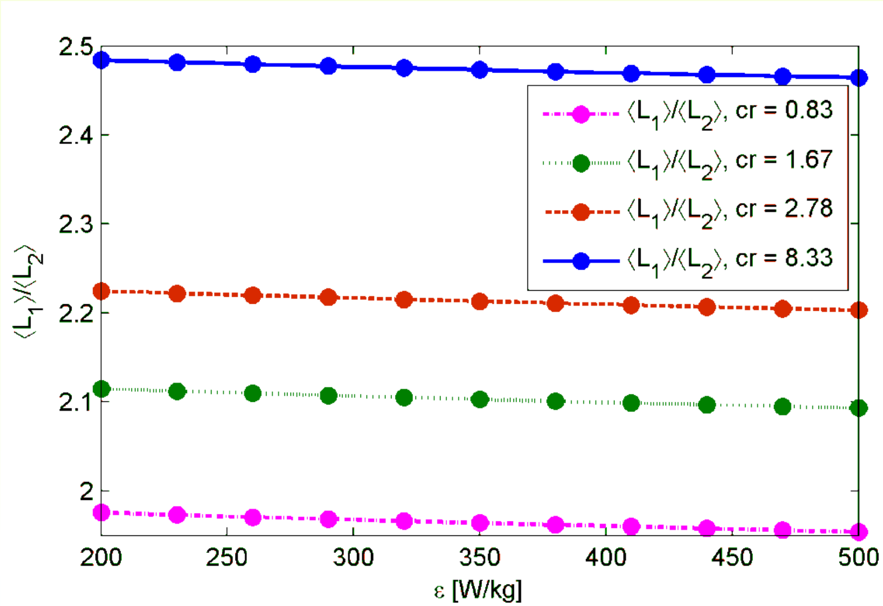


Figure 3. Effects of cooling rate on particle shape **[2]**

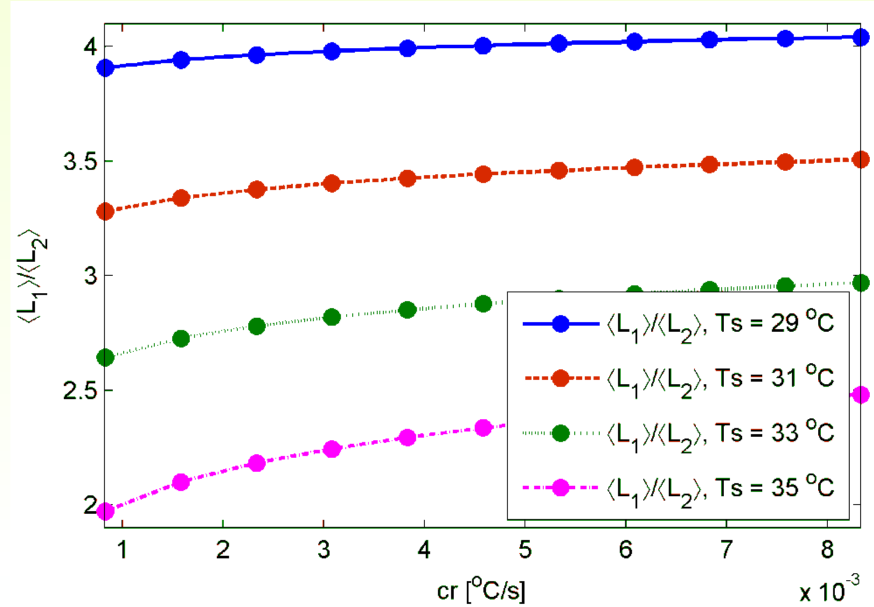


Figure 4. Effects of seeding temperature on particle shape **[2]**

Figure 5. Realizable interval of particle shape

[2] Szilagyi , B., Lakatos, G.B., ***Batch cooling crystallization of plate-like crystals: A simulation study,*** Per. Pol. – Chem. Eng**,** *DOI: 10.3311/PPch.7581*

M-PB: Crystallization of rod-like crystals

- ***Phenomenon of rod-like particle crystallization***

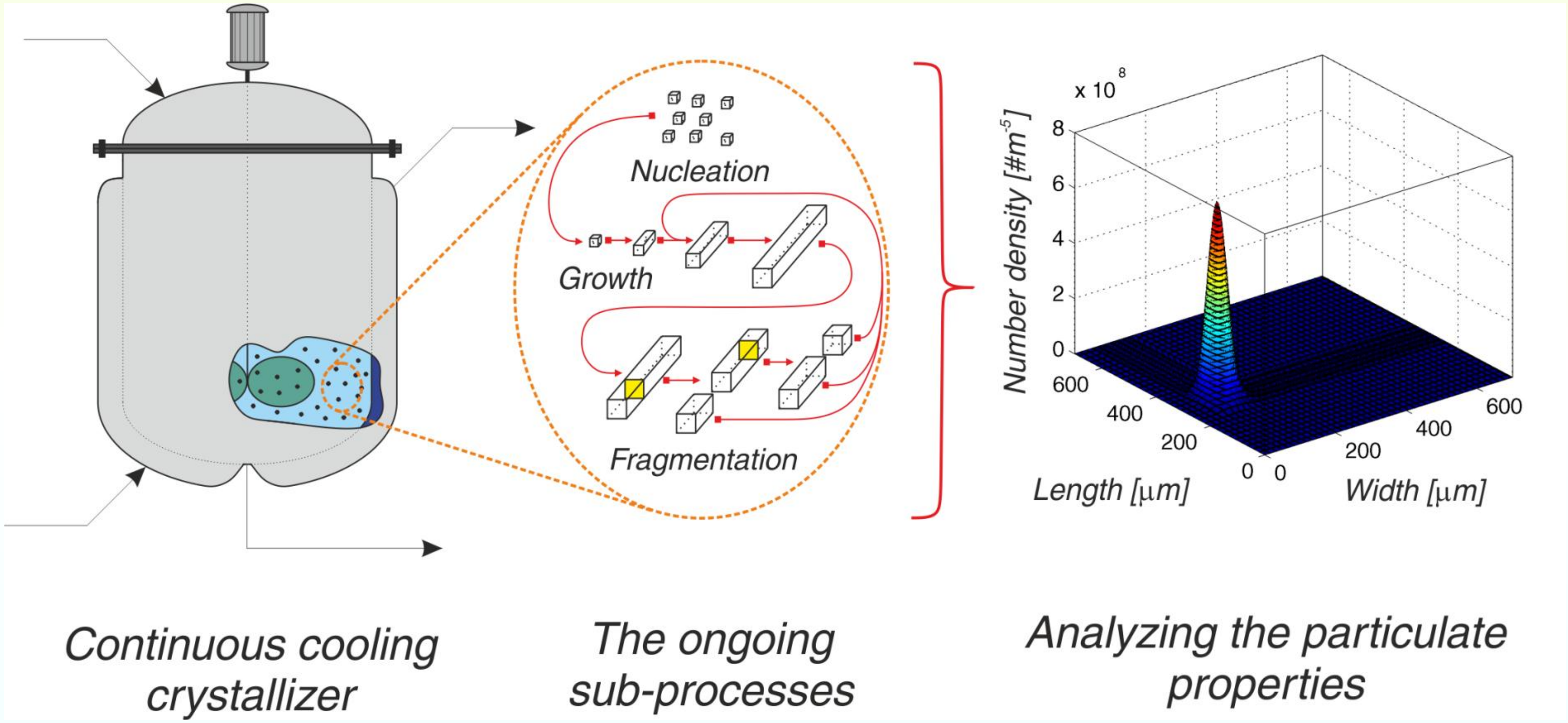


Figure 6. The rod-like particle crystallization

M-PB: Rod like crystallization: A “simple” PB model

- ***Mathematical model (the population balance only)***

$$\frac{\partial n(L_1,L_2,t)}{\partial t}+\frac{\partial[G_1 n(L_1,L_2,t)]}{\partial L_1}+\frac{\partial[G_2 n(L_1,L_2,t)]}{\partial L_2}=\frac{1}{\tau}[n_{in}(L_1,L_2,t)-n(L_1,L_2,t)]$$

$$+B_p(t)\delta(L_1-L_n,L_2-L_n)-k_{br}\int_0^{L_m}\int_0^{L_m} b_{br}^1(\lambda_1,L_1)b_{br}^2(\lambda_2,L_2)L_1^\beta L_2^\gamma n(L_1,L_2,t)d\lambda_1 d\lambda_2$$

$$+k_{br}\int_0^{L_m}\int_0^{L_m} b_{br}^1(L_1,\lambda_1)b_{br}^2(L_2,\lambda_2)\lambda_1^\beta \lambda_2^\gamma n(\lambda_1,\lambda_2,t)d\lambda_1 d\lambda_2$$

With the appropriate initial and boundary conditions

+++ Kinetic equations for primary nucleation, growth and particle-impeller collision breakage

+++ Heat and mass balance equations

+++ Solution of model-equations

Conclusions

- ***In the last months 1 article was accepted in an ISI indexed journal – Periodica Polytechnica – Chemical Engineering and***

- ***In the last months 1 article was submitted to an ISI indexed journal – Powder Technology***

- ***Future plans (for the following 2 months):***

    - ***Finalize the codes and write the manuscript for the 2D finite volume PBE solution***

    - ***Prepare the simulation data for the heat effect manuscript***

Thank you for your attention!