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Soft sensors for a batch crystallization process

Lucas Brivadis*, Vincent Andrieu, Élodie Chabanon, Émilie Gagnière, Noureddine Lebaz and Ulysse Serres

LAGEPP, CNRS UMR 5007, Université Claude Bernard Lyon 1, Lyon, France

* lucas.brivadis@univ-lyon1.fr

Introduction

- **Context:** During a batch crystallization process, the online control and estimation of the **Particle Size Distribution** (PSD) is critically important for the industry.
- **Problem:** No online sensor can measure the PSD.
- **Objective:** To build an online soft sensor that estimates the PSD, based on either the **solid concentration** or the **FBRM® technology**.
- **What is new?** No use of a nucleation model.

Model of the crystallization process

Hypothesis:

- $[t_0, t_1]$: Process duration.
- $[x_{\min}, x_{\max}]$: **Spherical crystals** radius range.
- $z(t, \cdot)$: PSD at time t .
- $G(t)$: **Growth kinetic** (McCabe hypothesis).
- $u(t)$: **Nucleation** at x_{\min} .

Population Balance Equation:

$$\begin{cases} \partial_t z(t, x) = -G(t) \partial_x z(t, x) \\ z(t_0, x) = z_0(x) \\ z(t, x_{\min}) = u(t). \end{cases}$$

Measurement : The solid concentration (up to some constant):

$$y(t) = \int_{x_{\min}}^{x_{\max}} z(t, x) x^3 dx.$$

How to estimate the state z from the measurement y ?

Luenberger original idea

Two steps strategy:

- 1 Estimate a function Tz of the state.
- 2 Invert this mapping T .

Designing an online soft sensor (Luenberger-like observer)

Step 1: Estimation of Tz . Consider, for $\lambda < 0$,

$$\dot{\zeta} = \lambda \zeta + y, \quad \zeta(t_0) = \zeta_0.$$

How to have $(\zeta - Tz) \xrightarrow[+\infty]{} 0$? It is sufficient to satisfy

$$\frac{dTz}{dt} = \lambda Tz + y.$$

For the solution a of some PDE, one can choose

$$Tz(t) = \int_{x_{\min}}^{x_{\max}} a(t, x) z(t, x) dx.$$

Step 2: Inversion of T ?

Tikhonov regularization method

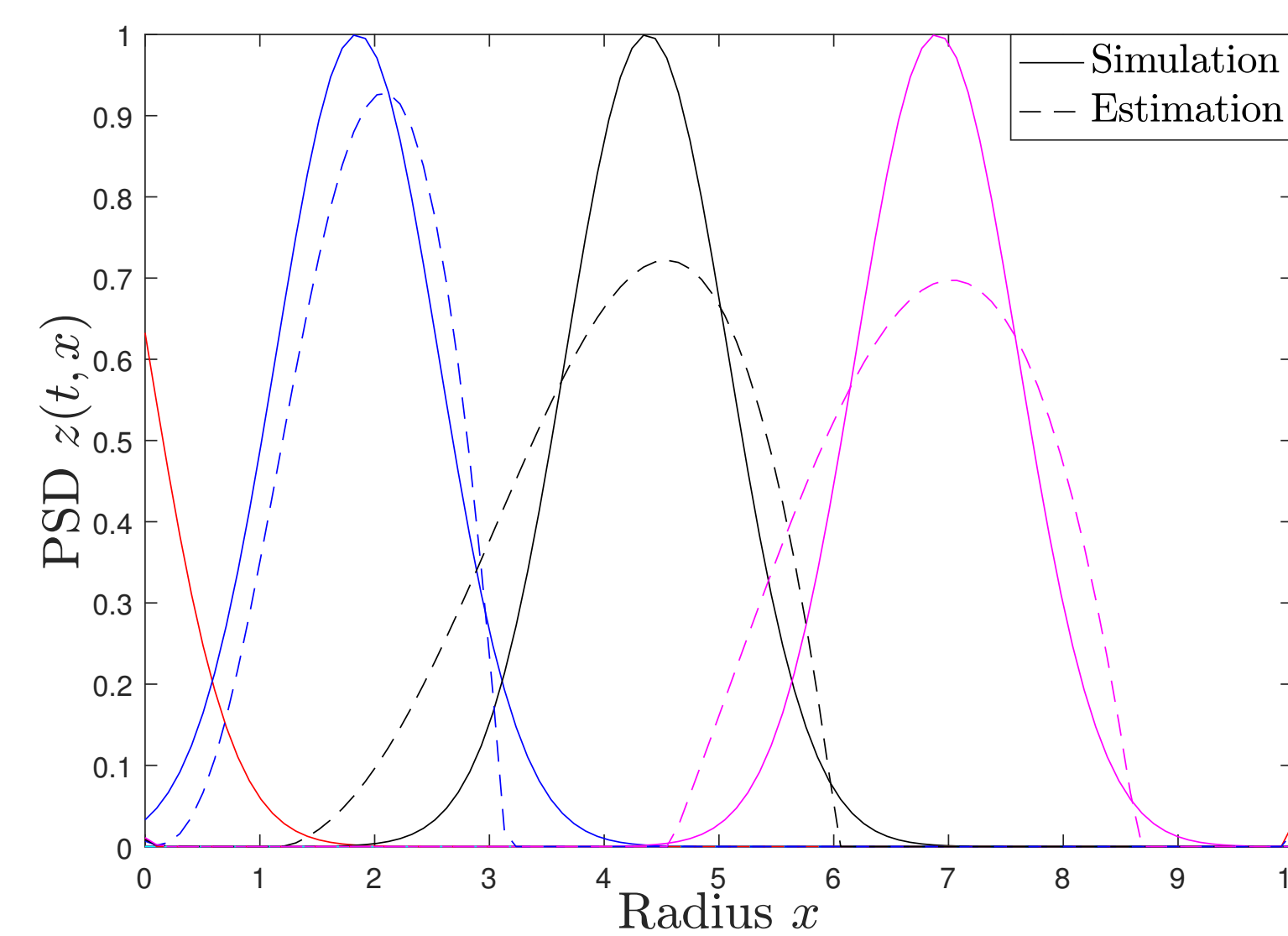
▪ **Problem:** Numerically estimate the solution of

$$\operatorname{argmin}_{\hat{z}(t)} \|T\hat{z}(t) - \zeta(t)\|_2^2$$

▪ **Idea:** Add a regularization term (**measure confidence**):

$$\operatorname{argmin}_{\hat{z}(t)} \|T\hat{z}(t) - \zeta(t)\|_2^2 + \delta^2 \|\hat{z}(t)\|_2^2$$

From solid concentration to PSD



Soft sensor based on the solid concentration with $\delta = 0.05$

Limits of the soft sensor:

- Need an estimation of the growth kinetic G .
- Choice of δ .
- Proof that y is not sufficient to determine z uniquely (**no injectivity**).
- Need a new physical sensor.

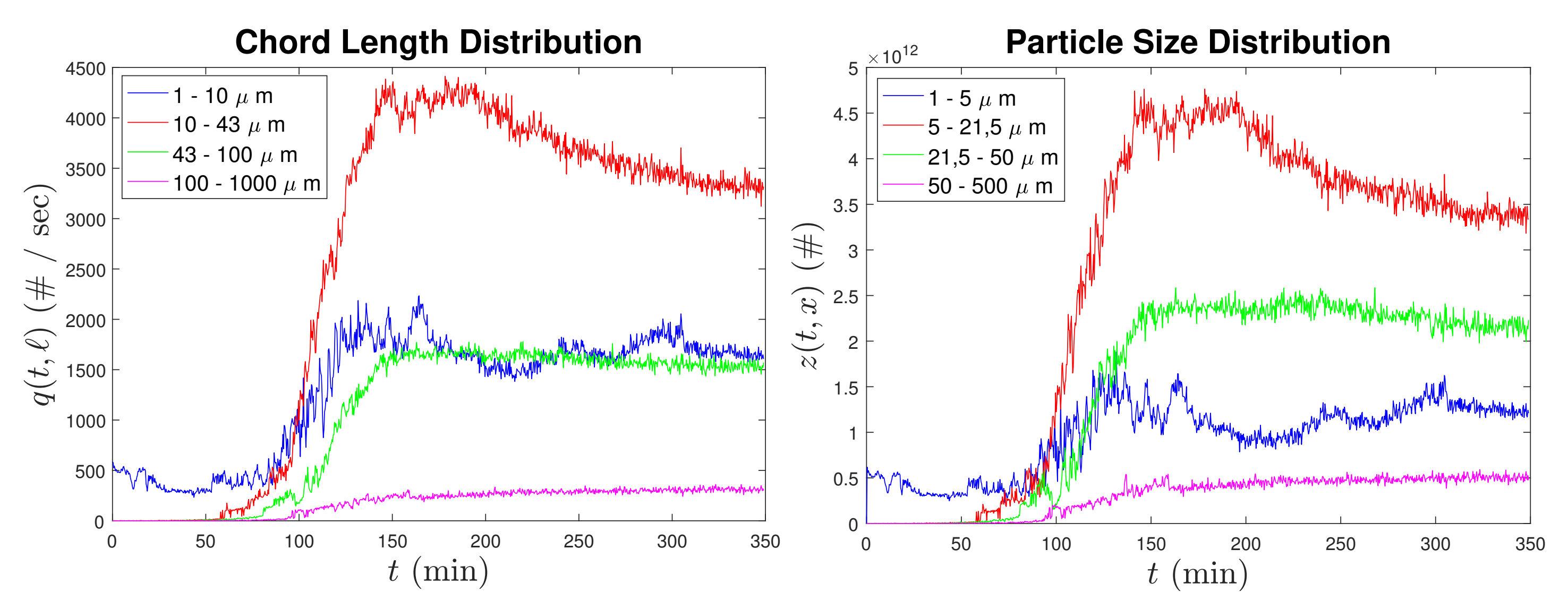
Model of the FBRM® technology

The probe uses a focused laser beam that scans across the particles. We model the measure as the **Chord Length Distribution** (CLD):

$$q(t, \ell) = C \int_{x_{\min}}^{x_{\max}} k(\ell, x) z(t, x) dx.$$

- $k(\ell, x)$ can be determined through a probabilistic analysis.
- C is an unknown constant. The solid concentration can be used to estimate C .
- One can apply the Tikhonov method directly on q , without using a soft sensor.
- Proof that q is sufficient to determine z uniquely (**injectivity**).

From CLD to PSD



Conclusion

- We propose two new soft sensors for the online estimation of the PSD in a batch crystallization process.
- The first one is based only on the solid concentration. This method has been tested on simulations. For better results, we prove that a new sensor is required.
- The second one is based on a mathematical modeling of the FBRM® technology, and has been experimentally tested. It allows to reconstruct the PSD from the CLD, both numerically and theoretically.

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