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Deterministic and Stochastic Modelling Concepts Suitable for Online Control of Industrial Reactors

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Highlights

- Fast Monte Carlo approach was developed for simulation of emulsion copolymerization.
- Kriging-based surrogate was used to eliminate stochastic nature of Monte Carlo method.
- The developed model allows prediction of molecular architecture for online optimisation.

1. Introduction

Past decades witnessed efforts to implement numerous advanced monitoring, optimization and control techniques in order to shift various productions from recipe-based to state-based operations, i.e. to allow for simultaneous optimization and control of the production in real time. This can be done using nonlinear model predictive control (NMPC) systems, which rely on a robust, precise and computationally fast mathematical model of the system. Various models suitable for online process control are typically based on a set of ordinary differential equations (ODEs), so they are only capable of controlling properties in continuous systems. However, there are complex systems (such as emulsion copolymerization, which we use as a case study), for which deterministic approaches cannot predict some valuable properties (e.g., detailed molecular architecture) or fail altogether due to underlying assumptions (separate particles cannot be treated as a continuous phase).

Stochastic Monte Carlo (MC) methods as an alternative to ODE-based models can provide detailed predictions of distributed properties, however at the expense of high computational time [1], which makes them unsuitable for the use in NMPC. Moreover, NMPC requires models based on deterministic equations in contrast to stochastic MC and MC predictions inherently contain statistical error, which is highly undesirable in online control. This issue can be solved by using surrogate modelling approaches.

2. Methods

Our system of interest is a seeded semi-batch emulsion copolymerization in monomer-starved regime with two water-soluble and two water-insoluble monomers. For such a complex system, we developed a rationally reduced model for NMPC based on 21 ODEs. This model is in agreement with 15 lab-scale experiments in conversion, solid content and number-average molecular weights of the product. The model-based NMPC system has been tested in various scenarios of online optimization at BASF pilot plant reactor [2] and shows promising potential for energy savings. For predicting extended properties, we implemented a hybrid MC model, which benefits from concentration profiles rapidly pre-calculated by ODE-based model and, consequently, saves a significant amount of computational time. Our 4-comonomer MC model is capable to simulate several hours of batch real time in only few seconds on a standard desktop PC, so it meets requirements on computational speed for NMPC. However, its use in NMPC is complicated due to its nondeterministic basis and statistical error.

For employing MC models in NMPC, we suggest using surrogate modelling, namely the Kriging model based on radial basis functions centred on testing values [3]. Choice of the testing values and incorporation of hybrid MC and surrogate model into NMPC is described in Figure 1.

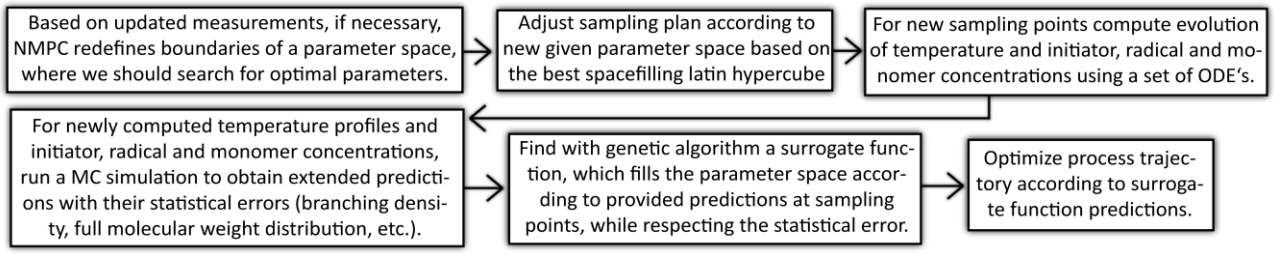

Figure 1. Incorporation of models into online NMPC, which assumes an existing surrogate function based on offline optimisation.

3. Results and Discussion

The deterministic (ODE) and stochastic (MC) models give reasonable agreement with experimental data as can be seen in Figure 2 (top graphs). The Kriging-based surrogate trained on the MC outputs (Figure 2, bottom) provides prediction of weight-average molecular polymer weight M_w in a functional form, which can be constructed in less than 10 seconds and its deviation can be adjusted to MC statistical error.

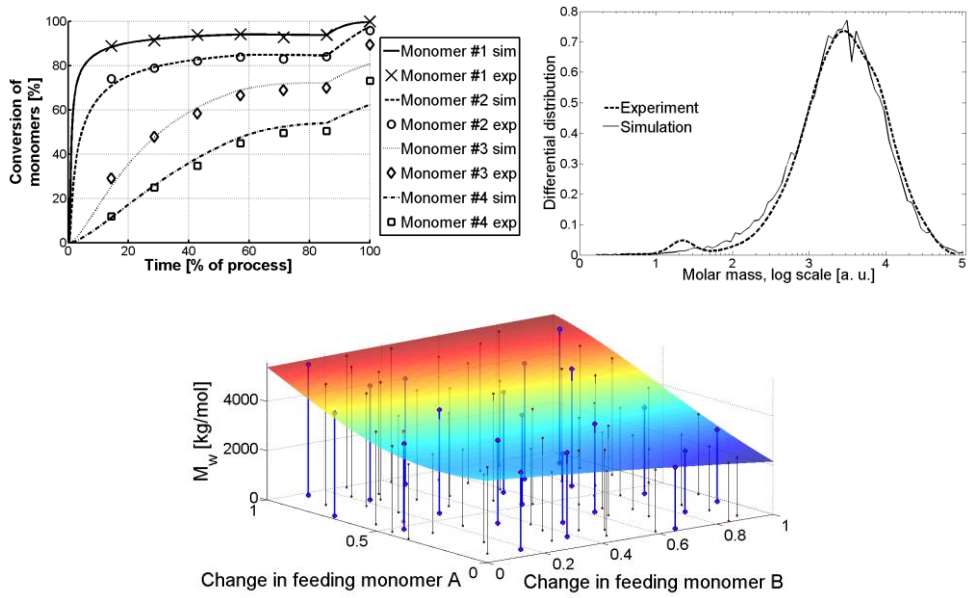

Figure 2. Top: Monomer conversions and full molecular weight distribution predicted by hybrid MC model in comparison with plant data. Bottom: Kriging-based interpolation (surface) of 40 MC outputs (black lines) compared to 20 testing MC outputs (blue lines).

4. Conclusions

We developed hybrid Monte Carlo model enabling very fast dynamic simulation of industrial pilot plant emulsion copolymerization reactor in a good agreement with experimental data. Kriging-based surrogate was trained on the hybrid MC model to minimize its statistical error and to approximate stochastic MC method by a functional form suitable for NMPC. Combination of hybrid MC and surrogate modelling may enable online control of complex properties in many different systems.

References

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Keywords
Model-based predictive control; Emulsion copolymerization; Monte Carlo simulation; Surrogate modelling.