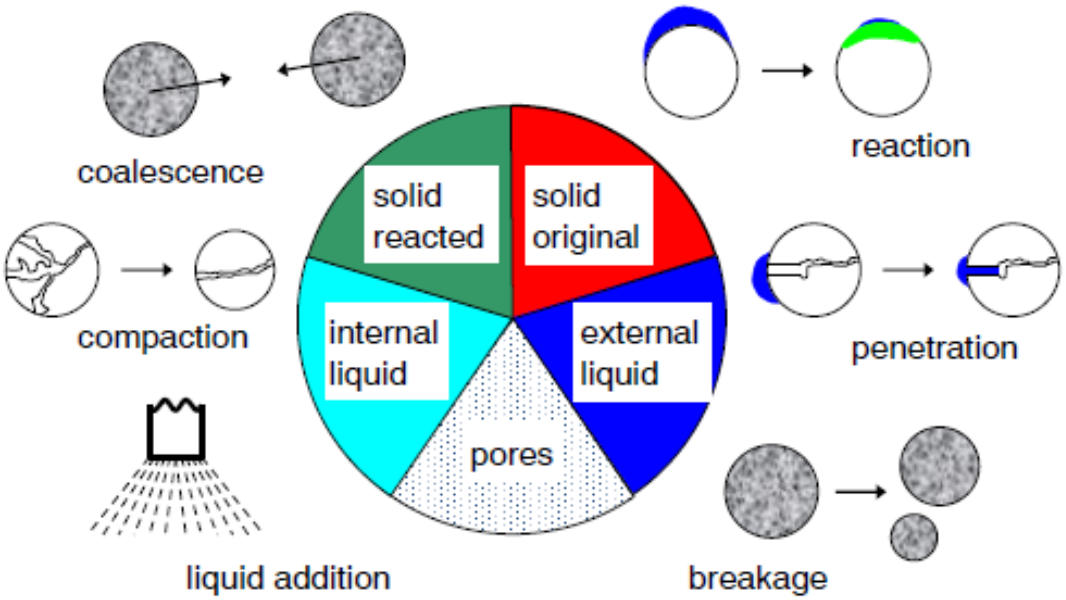
user story

Accounting for uncertainties in advanced model parameter estimations

application to granulation processes



Mathematical models are nowadays an integral part of process design and optimisation. The model can be of empirical nature, based on first principles or a mixture of both. The complexity of models can vary from application to application. However, all models contain model parameters, and these needs to be estimated in one way or another.

THE CHALLENGE

Estimate unknown model parameters in a complex granulation model

THE SOLUTION

Apply in-house parameter estimation methodology

THE RESULTS

parameter estimates incl. 1D marginals, 2D marginals

For example, modelling of particle formation processes such as granulation, crystallisation or flame synthesis is often based on the solution of population balance models. Population balance models are used to track the properties of entities such as particles, bubbles or bacteria. The type of accounted properties can be anything from particle diameter to bubble composition and age of a bacterium. While population balance model frameworks are very powerful, due to the versatility of accounting for all kinds of process phenomena as well as providing a wealth of model prediction such as the particle size distribution, their complexity means that the models often contain a number of empirical and semi-empirical model parameters. In fact, this is true for any kind of model.

THE CHALLENGE

The kinetic model parameters of a multidimensional population balance model for a granulation process were unknown and needed to be determined by solving the inverse problem.

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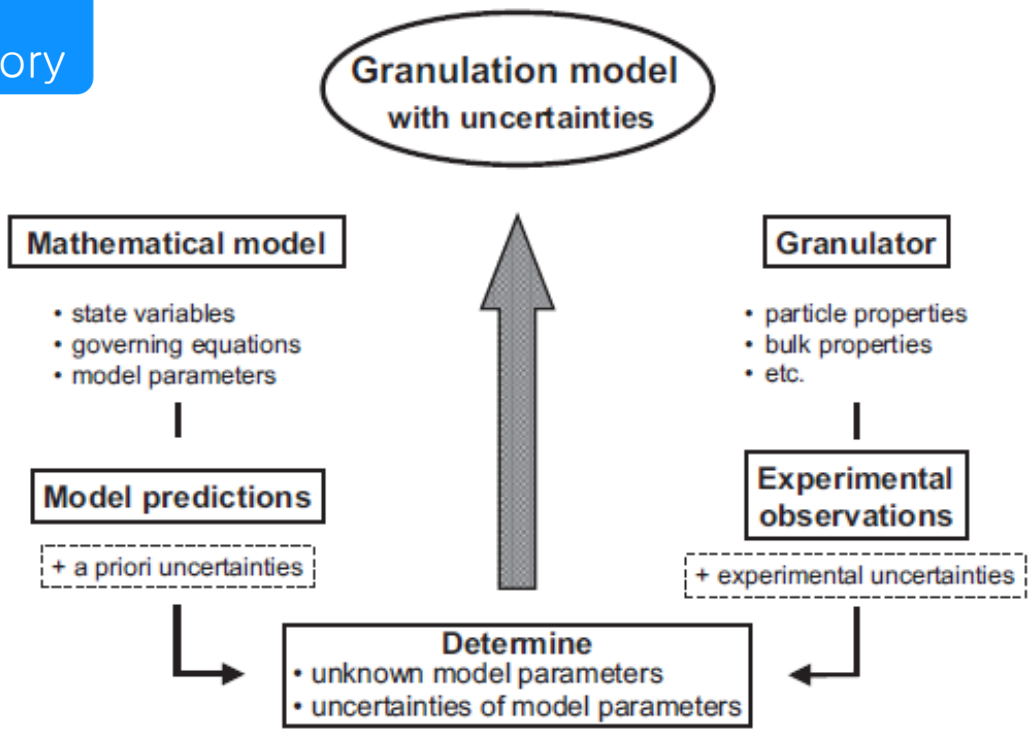
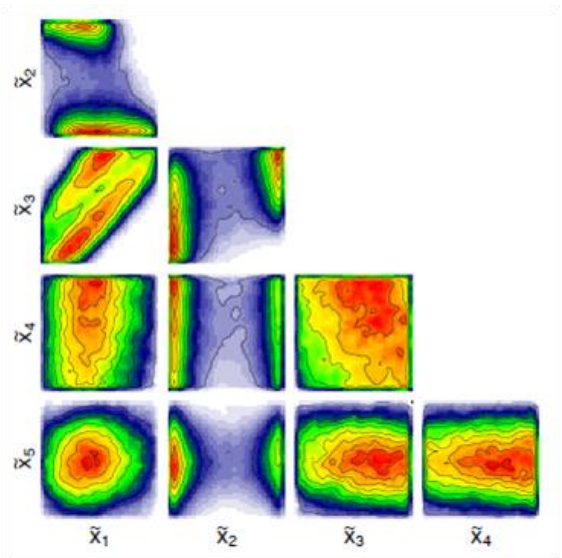


Above: Summary of the challenge

THE SOLUTION

The strategy for estimating the parameters makes use of experimental observations including their uncertainties along with evaluations of the complex granulation model, which are computational expensive. Firstly a region where the parameter set is likely to be found was identified using a search based on low-discrepancy series. Using this response surface, a model was set up in this region for the various process conditions and exploited by estimating the unknown parameters with a Bayesian approach.



Above: 2D marginal distributions of the five kinetic parameters of the multidimensional population balance model for a granulation process

THE RESULTS

As a result the parameter values could be deduced along with credibility regions. In addition, one- and two dimensional marginal distribution for the five unknown parameters were extracted, allowing the identification of multimodal distributions as well as correlations between the different parameters.

With the newly derived parameters it is now possible to solve the model for the process of question. The knowledge about the uncertainties in each parameter reveals also the areas for further model advancement. This could be the running of further experiments to improve the accuracy of the parameter estimation. Better process understanding and higher accuracy in the model predictions can also be achieved by improving particular aspects/submodels of the model framework.

APPLICATION AREAS

•Modelling of particle formation processes

•Any model with parameters

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