

Model-based state estimation of chemical processes using gray-box models

The use of model-based controllers in the chemical industry has increased significantly in recent years. The aim is to improve the control quality and thus to produce with constant quality, for example with optimal use of energy. For continuous systems, software tools have been established for these tasks that support the developer in data acquisition, modeling, and controller design. These tools usually use linear models that are identified with the help of tests in the plant and are only valid around a fixed operating point.

In specialty chemicals, small quantities are often produced in batch plants. The behavior of a batch process with steps such as filling, heating, reaction etc. can generally no longer be described by a linear model. To optimize a batch process, therefore, non-linear model-based methods (Nonlinear State Estimation, NMPC: Nonlinear Model Predictive Control) are used. In contrast to linear continuous processes, there are no established tools for batch processes to use model-based methods to control the processes.

Another difference between continuous and batch processes is that exclusively data-driven modeling is only possible to a limited extent due to the often limited availability of data. Therefore, hybrid modeling ("gray box modeling") as a combination of balance equations and data-driven components is a possibility to model batch processes.

For the application of methods based on non-linear models, knowledge of the state variables of the system is required. Since there are usually no real measurements for these variables, state estimators are to be used in this thesis, which determine the state variables via a hybrid process model.

Work packages

- Review of existing literature on the subject of condition estimation and gray box modeling of chemical processes, including the preparatory work carried out at Evonik
- Familiarization and testing of a tool that enables the industrial implementation of NMPC
- Optimization of an existing gray box model, especially the black box part, with the help of existing process data
- Implementation and testing of a non-linear model-based state estimation with a gray box model in a simulation environment

Requirements

- Programming skills (MATLAB)
- Interests in applied control / nonlinear model-based state estimation
- Interests in modelling of chemical processes (no detailed knowledge necessary)

Other

- Start: March 1st, 2022
- Duration: 6 months
- Location: Hanau-Wolfgang
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