Model based optimal design of dynamic experiments in gray-box and black-box modeling of fermentation processes

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The modeling of the fermentation of bacteria with the goal to produce the sporulated form of the micro-organism is a challenging task. This is firstly, because of general difficulties to describe the vast biochemical reaction network occurring inside of the cell. These metabolic reactions describe among others the substrate conversion to biomass and the production of messenger substances, that are used by the micro-organisms to communicate the initiation of sporulation. Secondly the sporulation process itself is also difficult to describe as it occurs over different stages in which the bacteria structurally change. [1] Because of these challenges a promising approach is the use of data-based machine learning models to describe the mentioned phenomena.

When using data-based models the deliberate acquisition of training data is a key aspect for prediction accuracy. Therefore, in this work different methods for designing experiments are compared like amplitude modulated pseudo-random binary sequences (APRBS) and model based optimal design of dynamic experiments as described by Körkel [2]. Here, the input trajectory is dynamically optimized to achieve a minimum parameter variance.

It can be shown that using gray-box models the prediction accuracy is favorable compared to black-box models due to the inclusion of first principles knowledge. Furthermore, the model accuracy can be improved by using an optimal experimental design strategy, that exploits knowledge about the model to find an input trajectory yielding maximum information about the underlying parameters.

References

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[2] Körkel, S. (2011). Optimum Experimental Design for Nonlinear Process Models. PAMM, 11(1), 719-720.