Automating Experimentation in Miniaturized Reactors

Operation of informative experiments has always been the necessity of an efficient process characterization at different stages of research and development. However, running experiments and collection of data is usually considered as a resource-demanding task. Hence, it is critically important to make educated designs for minimizing the number of required experiments. An unappropriated design of experiments (DoE) can easily end up with a waste of materials and resources for a small given information.

Application of different modeling techniques for DoE is to guarantee a high-level of information from every single one and move more towards the optimum experiments. This capability can be considered in different aspects of design of experiment for studying the effect of process variables, to design of the experimental operating condition which provides a similar process environment as the real-scale system in the lab-scale.

Model-based DoE is a category of DoE methods that is based on the integration of modelling techniques with statistical analysis. A Model-based DoE method benefits from the potential of mathematical modelling to predict the process behavior under various conditions. As the result, the proposed experiments are more focused on a set of target objectives. These objectives could be the identification of the key process variables, studying the process response to the change of environment, characterization of the interactions or even discrimination between some theories.

On the other hand, application of modelling approaches have been established for designing representative scale-down models for operation of the experiments. An ideal scale-down model has to provide a comparable process condition as the corresponding full-scale reactor to guarantee similar process behavior to the designed process variables. However, reaching such a design is usually a challenging task with respect to the limitations of different scales.

Considering the importance of presenting more robust and efficient DoE approaches, this thesis provides a comprehensive study on the application of model-based methods for design of optimum experiments. The studied topics cover different angles of the experimental design in miniaturized reactors including a framework to choose the values for the process variables and a method for design of a scale-down model for operation of the experiments.

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