A framework for a direct exploitation of available information in the online model-based redesign of experiments

Riccardo De-Luca[a], Federico Galvanin[b], Fabrizio Bezzo[a]

[a]CAPE-Lab   Computer-Aided Process Engineering Laboratory
Department of Industrial Engineering
University of Padova, via Marzolo 9, 35131 Padova, Italy

[b]Department of Chemical Engineering
University College London, Torrington Place, London WC1E 7JE, United Kingdom

MBDoE aims at designing a set of experiments yielding the most informative process data to be used for the parameter estimation of first-principles dynamic process models. According to the standard procedure described in literature [1], the experiment is generally designed offline; then it is carried out in the plant/lab, process measures are collected and parameter estimation is carried out only at the end of the experimental run: since the experiment is designed on the basis of the initial available parameter estimates, the progressive increase of the information resulting from the progress of the test is not exploited. In order to overcome this problem new techniques were proposed [2,3], where the information is exploited as soon as it is generated by the execution of an experiment by redesigning the experiment online through intermediate parameter estimations. This technique enables users to reduce the number of experimental trials needed to reach a statistically sound estimation of model parameters and results in a substantial reduction of time and costs. Nevertheless, this technique exhibits some limitations potentially hindering the effectiveness of the redesign procedure: on the one side, the time point at which redesigning the experiment is chosen "a-priori", without verifying whether enough information has indeed been collected to obtain an improvement in the estimation of the parameter value; on the other hand, the first design may be heavily affected by the initial parametric mismatch.

In order to overcome those problems a new strategy is here proposed. The main advantages is that a robust approach [4] is adopted within the online redesign procedure and, most importantly, a new design criterion based on the maximisation of a target profile of dynamic information is introduced. The methodology allows determining *when* to redesign the experiment in an automatic way, thus guaranteeing that a sufficient increase in the information content has been achieved before proceeding with the intermediate estimation of the parameters and the design of the experiment. Furthermore, the robust approach allows reducing the negative effects of the initial parametric mismatch. The effectiveness of the new experiment design techniques is demonstrated through a simulated case study.

References

[1] Franceschini G., Macchietto S., 2008, Model-based design of experiments for parameter precision: state of the art, *Chem. Eng. Sci.*, 63, 4846-4872.
[2] Stigter, J.D.; Vries, D.; Keesman, K.J., 2008 On adaptive optimal input design: a bioreactor case study. *AIChE J.*, 52, 3290–3296
[3] Galvanin F., Barolo M., Bezzo F., 2009, Online model-based redesign of experiment for parameter estimation in dynamic systems, *Ind. Eng. Chem. Res.*, 48, 4415-4427.
[4] Asprey S. P., Macchietto S., 2002, Designing robust optimal dynamic experiments, *J. Process Contr.*, 12, 545-556.