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# Real-time adaptive input design for the determination of competitive adsorption isotherms in liquid chromatography

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## 1. Abstract

The adaptive input design (also called online redesign of experiments) for parameter estimation is very effective for the compensation of uncertainties in nonlinear processes. Moreover, it enables substantial savings in experimental effort and greater reliability in modeling.

We present theoretical details and experimental results from the real-time adaptive optimal input design for parameter estimation. The case study considers separation of three benzoate by reverse phase liquid chromatography. Following a receding horizon scheme, adaptive D-optimal input designs are generated for a precise determination of competitive adsorption isotherm parameters. Moreover, numerical techniques for the regularization of arising ill-posed problems, e.g. due to scarce measurements, lack of prior information about parameters, low sensitivities and parameter correlations are discussed. The estimated parameter values are successfully validated by Frontal Analysis and the benefits of optimal input designs are highlighted when compared to various standard/ heuristic input designs in terms of parameter accuracy and precision.

## 2. Introduction

Model-based Optimal Experimental Design (OED) aims to maximize the information content of experiments for model development purposes. It has

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