Accepted Manuscript

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

Author: Tilman Barz Diana C. López C Mariano Nicolás Cruz Bournazou Stefan Körkel Sebastian F. Walter

PII: S0098-1354(16)30229-0

DOI: http://dx.doi.org/doi:10.1016/j.compchemeng.2016.07.009

Reference: CACE 5510

To appear in: Computers and Chemical Engineering

Received date: 10-4-2016 Revised date: 5-6-2016 Accepted date: 3-7-2016

Please cite this article as: Tilman Barz, Diana C. López C, Mariano Nicolás Cruz Bournazou, Stefan K*ddoto*rkel, Sebastian F. Walter, Real-time adaptive input design for the determination of competitive adsorption isotherms in liquid chromatography, <![CDATA[Computers and Chemical Engineering]]> (2016), http://dx.doi.org/10.1016/j.compchemeng.2016.07.009

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



ACCEPTED MANUSCRIPT

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

Tilman Barz^a, Diana C. López C. ^b, Mariano Nicolás Cruz Bournazou^c, Stefan Körkel^d, Sebastian F. Walter^e

^aAIT Austrian Institute of Technology GmbH, Giefinggasse 2, 1210 Wien, Austria
^bTechnische Universität Berlin, Chair of Process Dynamics and Operation, Str. des 17.
Juni 135, 10623 Berlin, Germany

^c Technische Universität Berlin, Institute of Biotechnology, Department of Bioprocess Engineering, Ackerstr. 71-76, D-13355 Berlin, Germany

^d University of Mannheim, School of Business Informatics and Mathematics, B6, 26, 68131 Mannheim, Germany

^e Universität Heidelberg, Interdisciplinary Center for Scientific Computing, Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

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

 $Email\ address: \verb|tilman.barz@ait.ac.at| (Tilman\ Barz)$

Preprint submitted to Elsevier

July 29, 2016

^{*}Corresponding author

Download English Version:

https://daneshyari.com/en/article/6595117

Download Persian Version:

https://daneshyari.com/article/6595117

<u>Daneshyari.com</u>