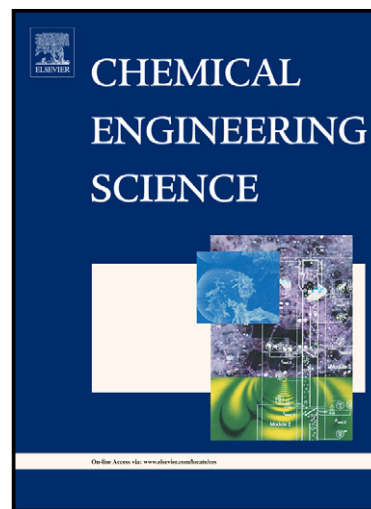


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# Robust design of optimal solvents for chemical reactions – A combined experimental and computational strategy

Teng Zhou<sup>a</sup>, Zhaoxian Lyu<sup>b</sup>, Zhiwen Qi<sup>b</sup>, Kai Sundmacher<sup>a,c,\*</sup>

<sup>a</sup>*Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, D-39106 Magdeburg, Germany*

<sup>b</sup>*Max Planck Partner Group at the State Key Laboratory of Chemical Engineering, East China University of Science and Technology, 130 Meilong Road, 200237 Shanghai, China*

<sup>c</sup>*Process Systems Engineering, Otto-von-Guericke-University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany*

\**Corresponding author: Tel.: +49 391 6110 350; Fax: +49 391 6110 353*

*E-mail address: sundmacher@mpi-magdeburg.mpg.de*

## Abstract

Solvents can have significant effects on chemical reactions, however, their huge number makes the selection very difficult and costly. This work presents a systematic method for the design of reaction solvents. Kinetic models are built by correlating experimentally determined reaction rate constants in a small set of known solvents with corresponding solvent theoretical descriptors determined from quantum chemical calculations. Optimal solvents are then identified from the solution of an optimization-based molecular design problem. Besides the deterministic optimization, a robust solvent design framework is proposed to identify solvents that possess the best reaction performance under model uncertainties. The methodology is exemplified for a competitive Diels-Alder reaction with the objective of maximizing the production of the desired

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