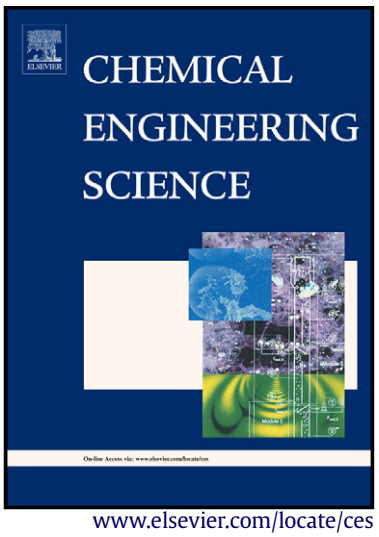

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Robust design of optimal solvents for chemical reactions – A combined experimental and computational strategy

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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