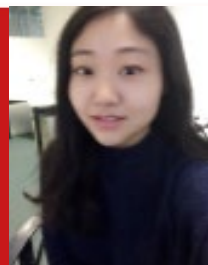


Spaciant Solvent Factory in ONE-FLOW: a combined modeling and experimental approach

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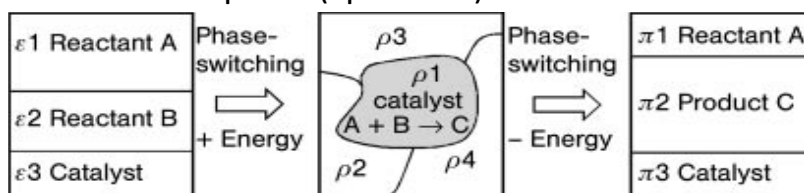


Introduction

Many green solvents are 'functional liquids' which allow interim creation or extinction of "fluidic spaces". They can co-exist, merge to provide homogeneous reaction conditions, separate to recycle catalysts and reactant, purify products, and remove waste by multiphase system. The Phd research topic explores the application of functional solvent systems in ONE-FLOW project, which aims to end-to-end green process design for pharmaceuticals, combining modeling methods with experimental validations.

Project summary

ONE-FLOW translates 'vertical hierarchy' of chemical multistep synthesis with its complex machinery into self-organising 'horizontal hierarchy' of a compartmentalized flow reactor system – a biomimetic digital flow cascade machinery with just one reactor passage. To keep horizontal hierarchy manageable, orthogonality among the consecutive reactions needs to be increased. The winning point of nature is to have invented catalytic cascades. ONE-FLOW will uplift that by enabling the best bio- and chemocatalysts working hand in hand. 4 synthetic flow cascades ('metabolic pathways') and 1 flow cascade driven by automated intelligence ('signaling pathway') will produce 4 Top-list 2020 drugs. 'The Compartmentalized Smart Factory' will develop organic, inorganic, and mechanical compartmentalization (nanoreactors). 'The Green-Solvent Spaciant Factory' will fluidically allow the use of interim reaction spaces (spaciant).



Project goals

1. One-pot process combining asymmetric organo- and biocatalytic reactions;
2. Allow the operation of two-step orthogonal catalysis in segmented micro-flow;
3. Screening and design solvent systems (e.g. TMS) for ONE-FLOW cascades;
4. Form nanoreactors and solvents' combination for a multitude of processing and purification tasks.

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