INTRODUCTION

- Self-optimisation combines an automated flow reactor with an optimisation algorithm for the autonomous identification of optimal operating conditions.
- Previous research was limited to the application of single objective optimisation algorithms such as SIMPLEX.
- In this work, we introduce a multi-objective optimisation framework which is based on machine learning.
- The algorithm learns the response surface of the chemical reaction system and uses surrogate models to reduce the number of expensive chemical experiments.

EXPERIMENTAL SETUP

- The experimental system is fully automated and experiments were designed and executed autonomously over night.
- The performance of the approach is illustrated by a four parameter optimisation of space-time-yield and E-factor of the nucleophilic aromatic substitution of 2,4-difluoronitrobenzene with morpholine in a microfluidic reactor.

RESULTS AND DISCUSSION

- Initially, 20 experiments were designed by a min-max Latin hypercube design and executed.
- Then, 48 experiments were designed sequentially by the TSEMO algorithm. During this process, the machine learning models were consistently updated.
- The experimental results converged to a dense Pareto front consisting of 27 points.
- The Pareto front dominates the complete initial data set. This means that for every point in the initial data set, one can find a point in the Pareto front, which outperforms the given point in both objectives.

CONCLUSION AND OUTLOOK

- The result emphasizes that automated self-optimising systems can identify optimal operating condition with respect to economic and environmental objectives with a minimum of experimental effort.
- The machine learning approach is capable of describing and optimising the reaction system efficiently.
- The Pareto front provides valuable inside about the inherent trade-off between economic and environmental objectives.