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Machine learning meets continuous flow chemistry: Automated optimization towards the Pareto front of multiple objectives

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ABSTRACT

Automated development of chemical processes requires access to sophisticated algorithms for multi-objective optimization, since single-objective optimization fails to identify the trade-offs between conflicting performance criteria. Herein we report the implementation of a new multi-objective machine learning optimization algorithm for self-optimization, and demonstrate it in two exemplar chemical reactions performed in continuous flow. The algorithm successfully identified a set of optimal conditions corresponding to the trade-off curve (Pareto front) between environmental and economic objectives in both cases. Thus, it reveals the complete underlying trade-off and is not limited to one compromise as is the case in many other studies. The machine learning algorithm proved to be extremely data efficient, identifying the optimal conditions for the objectives in a lower number of experiments compared to single-objective optimizations. The complete underlying trade-off between multiple objectives is identified without arbitrary weighting factors, but via true multi-objective optimization.