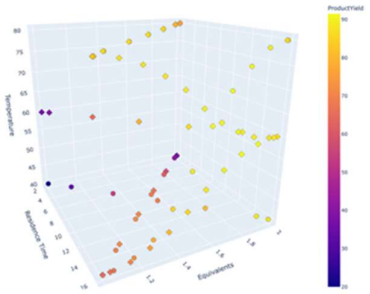
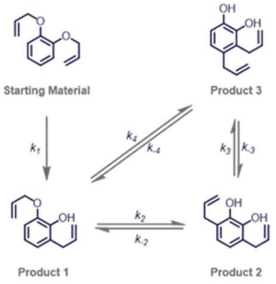
Printing kinetic data and microkinetic models in an automated lab

Reaction data is important to collect not only for theoretically understanding chemistry, but also for sustainably mass-producing chemicals for medicine, agriculture, and society in general. The AI for Science movement has seen progression towards more data-driven and modelling-based approaches, however application of ML in process development and scale-up has been limited by the availability of expensive to collect chemical reaction data. The development of automated transient flow methods integrated with machine learning has provided an efficient tool by which kinetic data can be collected efficiently and integrated directly with AI methods to automatically generate process insights and microkinetic models.

Through an integrated workflow of machine learning driven experimental planning, automatic data rich experimentation, automated data analysis, and automatic microkinetic model creation, we have drastically reduced the effort and time needed to produce robust kinetic insights. This integrated automated approach not only allows us to print kinetic insights for reactions we perform but also allows quantitative prediction for unseen reactions thanks to our transfer learning approach from our large in house data sets.





In this presentation, we discuss transient flow as an efficient data collection tool, our unique integrated workflow for kinetics, and a range of academic and industrial examples. We will also discuss new capabilities applied to different areas of chemistry and our latest machine learning developments.

SOLVE Chemistry is a London-based seed-stage start-up focusing on making chemical processes more efficient through autonomous high-throughput reaction data collection to construct AI reaction space models. SOLVE currently serves clients across the agrochemical, pharmaceutical, and fine chemical space.