Optimising Ag/Au Alloyed Nanoparticle Catalysts in Continuous Flow; Discrete vs. Continuous Variable Optimisation

Louis Greenhalgh with the Chamberlain Group at the University of Leeds iPRD lab
cm18lg@leeds.ac.uk

Skills 4 Scientists

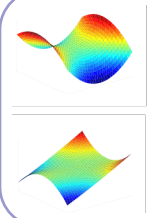
Sponsored by: optibrium, dotmatics knowledge solutions

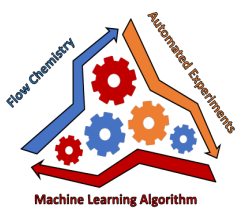
1. Introduction

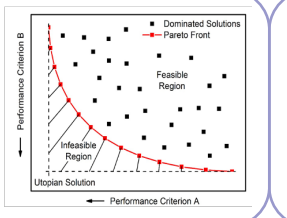
- **Nanoparticles** (NPs) have demonstrable utility as **catalysts** in many avenues of chemical production, due to their high energy surfaces and extremely high surface atom to volume ratios.
- **Continuous-flow reactors** provide a **scalable** way of manufacturing NP catalysts, with the potential for **self-optimisation** to increase **yield**, reduce **time**, **environmental & materials cost**, **human requirement** and the need for ***a priori*** chemical knowledge such as kinetics.
- Machine learning algorithms such as **Bayesian Optimisation** allow the determination of **global response curve minima**, while minimising the number of experiments required through **artificially-intelligent** decision-making.
- This project explores the benefits of optimising **continuous** over **discrete** variables in continuous flow synthesis and utilisation of these NP catalysts.

2. Self-Optimisation of Continuous-Flow Chemistry

- Continuous-flow reactors allow the automation of experiments. When combined with algorithmic self-optimisation to generate experimental conditions, this permits the effective exploration of large amounts of experimental space to find local and global optima.
- This is achieved using UV-vis on-line analysis of the generated products that creates a feedback-loop, using an optimisation algorithm with an "acquisition function" to efficiently choose the next conditions to test in order to most quickly reach the "global optimum" within the modelled system.
- This has the potential to expedite discovery and enhance research undertaken in synthetic laboratories, termed "High-Throughput Experimentation" (HTE).





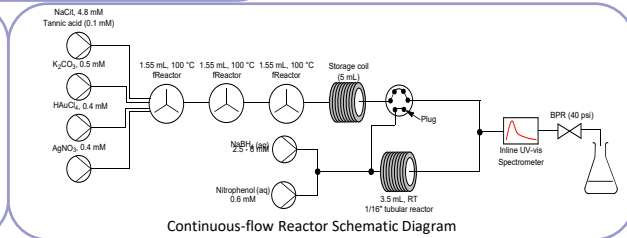


3. Bayesian Optimisation and System Modelling

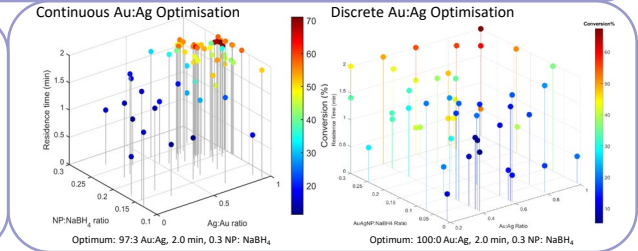
- Optimsation is termed "Bayesian" because previous evidence or "priors" are updated with new evidence on every iteration to produce a new surrogate model.
- Bayesian optimisation treats a system as a "Gaussian process" where the distribution of possible results is dealt with as an infinite array of gaussian functions.
- It uses a mean and covariance function to represent the data in a simplified "surrogate model" created from training data about a complex real-life system (such as our continuous-flow reactor).
- Every iteration of the algorithm produces a new surrogate model with a distribution closer to that of the true objective function, with the variance representing uncertainty – i.e. greater further from the training data.
- This allows the modelling of a real life system from a set of experimentally generated training-data which can be used to produce modelled experiments with varied values for the input conditions.

4. Discrete vs. Continuous Variable Optimisation

- The ratio of Au:Ag in the alloyed nanoparticles (synthesised using the Turkevitch protocol) was varied and optimised as a ***continuous variable*** along with residence time, reduction concentration with the objective of obtaining maximum conversion in a test reduction reaction using a Bayesian optimisation algorithm.
- This project will repeat these experiments but exploring the Au:Ag ratio of the NPs as a ***discrete variable*** with a variety of possible compositions to quantify the pros and cons of each approach.



Continuous-flow Reactor Schematic Diagram



Optimum: 97:3 Au:Ag, 2.0 min, 0.3 NP: $NaBH_4$

Optimum: 100:0 Au:Ag, 2.0 min, 0.3 NP: $NaBH_4$

AI³ Science Network+

UNIVERSITY OF LEEDS

PSDS PHYSICAL SCIENCES DATA-SCIENCE SERVICE

RSC INTEREST GROUP CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP