Self-Optimizing Process Control for the synthesis of fluorescent carbon quantum dots

Henry Rosier, Thomas Kretzschmar

HiTec Zang GmbH, Herzogenrath, Germany
henry.rosier@hitec-zang.de

Self-optimizing process control techniques have proven effective in enhancing the efficiency and quality of chemical reaction processes [1]. Continuous synthesis of carbon quantum dots (CQDs) within a microreactor can greatly benefit from optimized process control [2]. Due to their fluorescence and low toxicity, CQDs find applications in various fields, including electronics, catalysis, medicine, and pharmaceuticals [3].
This work focuses on the optimization of carbon nanoparticle synthesis in an automated, continuous microreactor system as an optimization example, with the aim of achieving maximum fluorescence intensity. The control of the process is handled by the LabVision automation system (HiTec Zang) while the optimization algorithm are implemented either in Python or Matlab.
Two different optimization algorithms, namely the SNOBFIT algorithm [4] and Bayesian optimization [5], are employed and their results are compared.

The system involved the reaction of citric acid and urea in continuous flow under varying conditions, with the synthesis parameters (flowrates, temperature, see fig. 2) optimized by the respective algorithms to attain the optimal fluorescence intensity. The outcomes of the optimization processes were then compared and evaluated.
The evaluation of the optimizations revealed a significant increase in the fluorescence of the particle dispersions, demonstrating the efficacy of the optimization algorithms in improving synthesis outcomes (see fig. 1). Moreover, the SNOBFIT algorithm, when compared to Bayesian optimization, demonstrated higher efficiency under the chosen hyperparameters. Importantly, the application of optimization algorithms enabled the experimental setup to autonomously improve the process conditions in over 100 experiments (see fig. 2).

Figure 1: Comparison between water (left), unoptimized (middle) and optimized (right) samples.

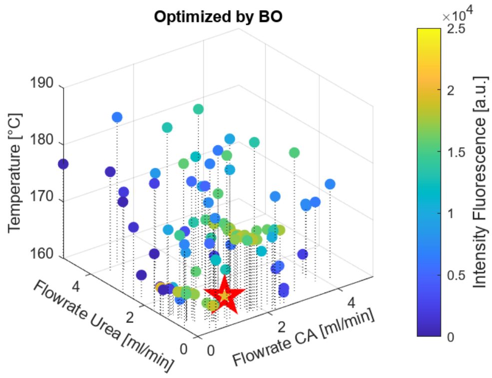

Figure 2: Plotting of iteratively measured fluorescence intensity in the choosen domain. Red star marks found optimum by Bayesian Optimization (BO).

This study sheds light on the potential of self-optimizing process control in enhancing the synthesis of carbon nanoparticles within microreactors, highlighting the effectiveness of the SNOBFIT algorithm in improving fluorescence intensity. The findings contribute to the development of more efficient and precise synthesis methods for carbon quantum dots with diverse applications in various fields. Taken this synthesis as an example, optimization algorithms can also applied to other systems and problems, which yields much potential for the chemical industry overall.

[1] Clayton et al., *React. Chem. Eng.*, **2019**
[2] McMullen et al., *Org. Process Res. Dev.*, **2010**
[3] Wang et al., Carbon quantum dots: synthesis, properties and applications, J*ournal of Materials Chemistry C,* **2014**
[4] Huyer et al., SNOBFIT -- Stable Noisy Optimization by Branch and Fit., *ACM Trans. Math. Softw. 35, 1–25,* **2008**
[5] Močkus, J., Bayesian Approach to Global Optimization, **1989**