An Multimodal Platform for Liquid-Liquid Partition Process Monitoring Aided by Computer Vision

Jiyizhe Zhang[1,2,3] **Alexei Lapkin**[1,2]

[1]*Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge CB3 0AS, United Kingdom* [2] *Innovation Centre in Digital Molecular Technologies, Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom* [3]*Department of Chemical Engineering, University of Manchester, Manchester M13 9PL, United Kingdom*

Correspondence to: Alexei Lapkin aal35@cam.ac.uk *Jiyizhe Zhang* jiyizhe.zhang@manchester.ac.uk

1. Introduction

Liquid-liquid partition coefficient is one of the fundamental properties for chemical separations [1], from screening new green solvents, to design downstream separation development. The traditional way to measure partition coefficient is by shake-up experiments, which consumes large volume of reagents and often time consuming. Online monitoring of liquid-liquid partition processes is even challenging which requires to take samples from both liquid phases. In recent years, lab automation and artificial intelligence have significantly advanced scientific discovery and accelerated chemical process development. It is hypothesised that with the access to advanced sensing technologies, lab automation and AI, it is possible to automate the measurements and online monitoring of liquid-liquid partition processes, meanwhile to get rich data from experiments.

2. Methodology

An automated experimental platform is developed for monitoring the partition process and measuring partition coefficients of liquid-liquid systems (Fig 1). The system mainly consists of an imaging system with a PC, a microchip and a pumping system. The imaging system consists of multiple detectors: a high-speed camera, two visible and near infrared hyperspectral cameras (SWIR and VNIR) and Raman spectroscopy. A glass microchip is mounted on a XYZ translation stage, and is connected to the pump system via PTFE tubing, which allows two liquid phases to be introduced and generate droplets to travel in the channel. The pumping system consists of a pump array for cleaning the channel with washing liquids. Two syringe pumps are applied for transporting the testing liquids into the channel.

The measurements begin with automated cleaning and rinsing of the microchip using ethanol and water. Then the high-speed camera starts capturing the fluid condition inside the channel, with a computer vision based classifier to detect droplet flow. This is followed by image analysis to extract slug sizes and moving velocity from the consecutive images. Based on this hydrodynamics information (i.e. drop sizes, drop velocity), imaging settings for hyperspectral camera is adjusted and the concentration measurements then start. The solute concentrations in each phase are determined through spectral analysis, where peak intensities are extracted and used to calculate partition coefficients.

The system is synchronised by Flab [2], which is a python-based framework allows for automating the experimental procedures.

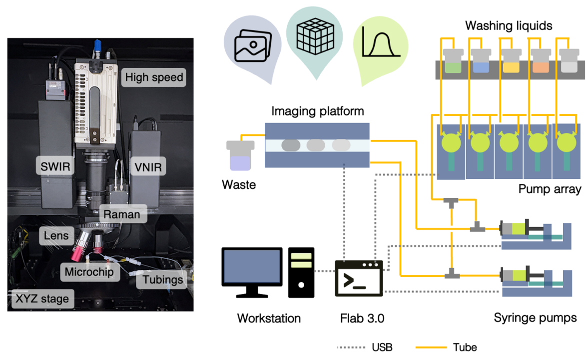

Fig. 1: Automated experimental setup design

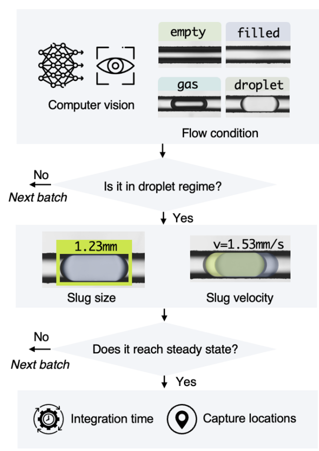

Fig. 2: Computer vision analysis

3. Results and discussion

3.1 Partition coefficient

Based on the experimental platform, we have successfully measured partition coefficients for various liquid-liquid systems, including dye molecules and metal-organic cages. Fig. 3 shows results of measuring partition coefficients at different locations as the droplet moving along the channel. The entire measurement is less than 20min per test system, significantly reduces human intervention.

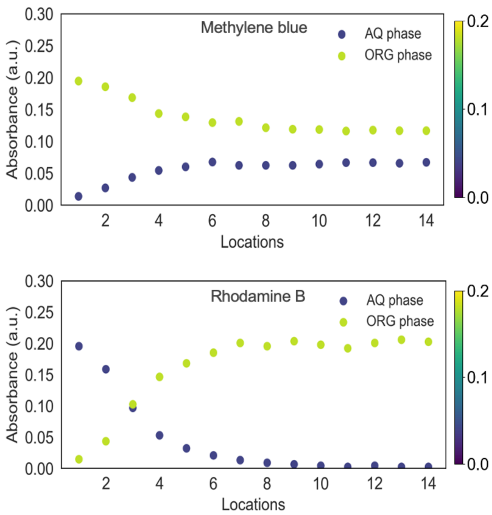

Fig. 3: Partition coefficient measurements at different locations

3.2 Dynamic concentration mapping

A dynamic online monitoring method was developed can achieve real-time mapping of concentration change during the liquid-liquid partition process. Fig. 4 shows concentration change at different locations, clear flow patterns of non-uniform mixing can be observed at droplet formation stage. The system can provide a label-free method to achieve real-time monitoring of the concentration change during liquid-liquid partition processes.

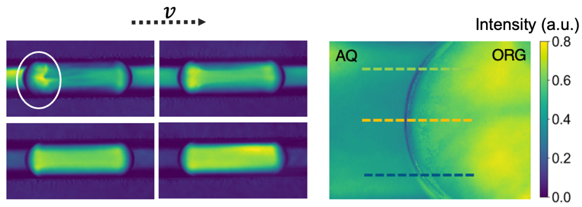

Fig. 4: Concentration maps droplets at different stage of partition process (methylene blue in octanol-water system)

Acknowledgments

This work was in part supported by EPSRC funded project EPSRC EP/W031019/1 "Bio-derived and Bio-inspired Advanced Materials for Sustainable Industries (VALUED)”. The work was enabled by Innovation Centre in Digital Molecular Technologies (iDMT) at Cambridge.

References

[1] Leo A, Hansch C, Elkins D. Partition coefficients and their uses. Chemical reviews. 1971, 71(6):525-616.
[2] Jose NA, Adesina P, Ballu K, Chitre A, Karan D, Katsarou A, Pomberger A, Zhai S, Lapkin A. A Universal Framework for Fast, Flexible and Fun(ctional) Autonomous Laboratories. Arxiv, 2024, 10.26434/chemrxiv-2024-990q0.