A Robotic Soft Matter Scientist: Transforming the Sustainability of Formulated Products

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Formulation of soft matter systems such as emulsions, gels, and suspensions is a core part of a wealth of industries aiming to develop products with desirable functional outcomes. However, product formulation is inherently challenging due to large design space, lots of trial-and-error, and numerous variable optimisations required to achieve ideal compositions. Automation and machine learning can be readily adapted to handling the repetitive processes and variable optimisations involved in materials discovery and product formulation.

Here, we take a 'frugal automation' approach to develop an automated system to provide greater flexibility to formulation and particle characterisation in place of standard inflexible, highly optimised and expensive kits. A method is developed to extract particle size distributions (PSD) from laser diffraction data using Mie scattering theory and computer vision (CV). Polystyrene microparticles with known PSD are used as test samples for diffraction analysis, and a compound optical microscope fitted with a complementary metal-oxide semiconductor (CMOS) camera is used to examine basic shape and size of the colloidal particles. This setup is then used to explore an applications-relevant model system. A benchtop experimental platform, comprising a UR5e robotic manipulator and Robotiq Hand-E adaptive gripper, is also under development for workflow automation.

Preliminary results from the CV-diffraction algorithm show that particle size can be predicted by directly comparing measured scattering intensity with theoretical scattering generated from an array of different particle sizes via a Mie theory optical model. Further improvements for the proposed system will focus on fully automating the synthesis, chemical analysis, and laser diffraction workflows. A machine learning model for hypothesis generation will also be considered for future iterations.

Keywords:
Automated formulation, particle characterisation, computer vision, particle size distribution