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The NIST Autonomous Formulation Laboratory: Solving Industrial Problems with Multifacility X-Ray and Neutron Scattering and AI

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Liquid formulations are ubiquitous, ranging from products such as deicing liquids to food/beverages and biologic drugs. All such products involve precisely tuned composition to enable engineered behaviors, whether that be a drug targeting high-pH tumor areas or a deicing fluid thinning at a specific shear rate so a plane takes off. These engineered responses often involve dozens of interconnected active components ranging from viscosity modifiers to dyes, preservatives, fragrances, etc. This complexity often precludes rational, physics-based optimization of product design in response to changing regulatory/sustainability drivers, for example. This talk will describe the Autonomous Formulation Laboratory, a project based at NIST that is capable of autonomously mixing liquids in arbitrary, n-dimensional composition space and characterizing the resulting formulation using x-ray and neutron scattering in combination with spectroscopy, rheology, and other measurements. This platform is driven by custom, highly flexible open source software that can be used to tackle a variety of different problems, from mapping the bounds of a specific, target phase with high accuracy to maximizing overall phase diagram exploration and everything in between. This talk will describe our development and application of the system to a variety of industrial formulation problems and recent efforts to provide highly robust, flexible data classifiers and data fusion approaches to make the most of multimodal data.

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