Proceedings of the Canadian Society for Mechanical Engineering International Congress 2022
CSME Congress 2022
June 5-8, 2022, Edmonton, AB, Canada

NUMERICAL MODELLING OF EMULSION FLOWS

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ABSTRACT

Emulsion-based products are widely encountered in our daily lives and industrial processes: food emulsions, pharmaceutical emulsions for drug delivery, emulsions in agriculture, and petroleum extraction. Emulsions are systems where one liquid is dispersed in the form of drops into another immiscible liquid with the addition of surfactant. An emulsion-based product design involves three major aspects: product formulation (ingredients), process conditions during manufacturing, and properties of the final product such as flavour, texture, and stability. The critical features of the final product are determined by the drop size distribution (DSD) of emulsion, which, in turn, depends on emulsion composition and the manufacturing process. Prediction and control of the DSD are crucial factors for successful emulsion-based product design and production.

In my research group, we create numerical techniques to perform in silico experiments to minimize trial-and-error time-consuming and costly laboratory experiments and, therefore, to develop sustainable and environmentally benign process design, scale-up and optimization of emulsion-based products. In this talk, I will demonstrate several of these techniques that can be used to study the emulsion flows on different levels of resolution and how the results of such models lead to a better understanding and prediction of the DSD. First, I will cover the fundamental studies of emulsion behaviour at the drop-resolved level that are performed with the diffuse interface lattice Boltzmann methods. The explanation of the methods along with its capabilities to perform direct numerical simulations (DNS) of immiscible flows will be shown. Second, the capabilities of the population balance equation (PBE) models to predict the DSD will be demonstrated. These PBE-based models allow consideration of the effects of dynamic conditions and system properties on the distribution of drop sizes. Third, the two approaches along with the machine learning techniques will be brought together to bridge the results of the DNS, PBE models, and experimental data to improve the prediction and control of the DSD which is one of the most important characteristics of emulsions.