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Multiscale Modeling of Food Emulsion Production Process

From Molecules to Mixing Equipment

By

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Most of the well-known food emulsions, such as mayonnaise, are made of a continuous water phase, a dispersed phase with high oil content, and surfactants that stabilize the oil drops. The Droplet Size Distribution (DSD) is the most important property of the emulsion since the structure, stability, taste, and color of the final product depend on the DSD. The DSD in turn depends on the emulsion composition, the type of process, and the operating conditions in which the production process operates. The production of emulsions is based on mixing the ingredients and applying enough mechanical energy to the emulsion to reach the desired DSD. During the emulsification process, the interfacial properties between dispersed and continuous phases play an essential role in the formation and stabilization of the oil droplets. Many food emulsions are stabilized by surface-active biopolymers that adsorb to droplet surfaces and form protective coatings. Some of these functional molecules are integral components of more complex ingredients used in food products (e.g., egg yolk). Although the egg yolk is recognized as one of the most widely employed emulsifiers for both industrial and home-made food emulsion preparation, many issues need to be addressed, especially the adsorption mechanism of egg yolk proteins at the oil-water interface and their emulsifier behavior. Experimental research concerning the emulsifying properties of egg yolk proteins has been hindered by the difficulties in extracting individual components from the complex matrix. Hence, within the multiscale framework, different time- and space- scales were investigated to describe the modeling approach from the molecular scale (oil-water interface) to the macro-scale (production device). The oil-water interfacial system, where the emulsifier is one of the most surface-active proteins from the egg yolk, so-called Apovitellenin I, was investigated using different molecular modeling techniques. The protein adsorption behavior at the interface and the interactions with other co-surfactants were described with the help of an atomistic model and statistical analysis. Then, a coarse-grained model based on the Dissipative Particle Dynamics (DPD) was employed to consider both the complex composition of the emulsion and the equilibration time required by macro-molecules to re-arrange at interfaces. Therefore, by combining the molecular methods with a thermodynamic model of

protein adsorption, a complete description of the interfacial system stabilized by protein surfactants was achieved. The approach employed eventually showed how these techniques can be linked together to predict equilibrium properties that are difficult to obtain experimentally for the system investigated. In addition, a scaling scheme for DPD simulations was applied to oil-water interfacial systems to study different coarse-graining levels, highlighting the advantages and limits of the proposed method for conserving the equilibrium properties of such systems. Another modeling method was also investigated, namely the Lattice Boltzmann Model (LBM). Although both DPD and LBM are successfully employed in modeling mesoscopic systems, they are conceptually different. Therefore, the two techniques were compared when dealing with immiscible fluids in presence of surfactants, with the aim of finding a possible link between the molecular and the continuum modeling approaches. Finally, at the macroscale level of description of the production device, Computational Fluid Dynamics (CFD) simulations were employed to properly describe the non-Newtonian dynamics of the emulsion and clarify the influence of the type of flow on the DSD, namely pure shear versus elongational. To describe the evolution of the DSD, the Population Balance Modeling (PBM) was employed, in which coalescence and breakage of oil droplets were taken into account by appropriate kernels, which depend on local flow conditions.