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Abstract

Food emulsions, such as mayonnaise, are made of a continuous water phase, a dispersed phase with a high content of oil, and a surfactant (i.e. the egg yolk for mayonnaise) that stabilizes 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.[1] 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. In particular, for the food emulsion investigated in this work, i.e. the mayonnaise, a typical mixing process is composed of two steps (Figure 1). First, the ingredients (mainly egg yolk, vinegar, oil, water, salt) are mixed together in large stirred vessels at a moderate rotational speed. Then, this premixed emulsion is finally fluxed into a high-shear device, commonly a cone mill mixer,[2] where the oil droplets undergo breakage until the final size distribution is reached. This last step is crucial to fine-tune the DSD, in order to determine the properties of the final product. A typical cone mill is constituted of a solid conical frustum rotor inside a slightly larger stator of the same shape, forming a small gap in which the emulsion flows and experiences high shear stresses, due to the high rotational speed of the rotor.

Within the multiscale framework, different time- and space- scales are investigated to describe the modeling approach for the macro-scale (cone mill) and the molecular scale (oil-water interface). Computational fluid dynamics (CFD) simulations are employed to properly describe the non-Newtonian dynamics of the emulsion, investigate the role of the pre- and post-mixing zones and clarify the importance of the type of flow, namely pure-shear versus elongational. In order to describe the evolution of the droplet size distribution, the Population Balance Modelling (PBM) is employed,[3] in which coalescence and breakage of oil droplets are taken into account by appropriate kernels, which depend on local flow conditions.

During the emulsification process, the interfacial properties between dispersed and continuous phases have an essential role in the formation and stabilization of the oil droplets.[1] Once the chemical composition of mayonnaise is determined, especially the biomolecules acting as surfactants, the interfacial tension between the two phases is directly computed with the help of atomistic techniques, such as Molecular Dynamics (MD) and Dissipative Particle Dynamics (DPD). This mesoscale approach also provides the surfactant adsorption kinetics and its molecular conformation at the interface, paving the way for a better understanding of the breakage and coalescence events of the oil droplets occurring in the production process. This information can be eventually transferred to the CFD-PBM simulations thus achieving a complete, general, and multi-scale model of the food emulsion production process.

This effort is carried out in the context of the VIMMP project (www.vimmp.eu), where the entire workflow will serve to devise a marketplace for generic multiscale and multiphysics simulations. The VIMMP project has received funding from the European Union's Horizon 2020 Research Innovation Programme under Grant Agreement n. 760907.
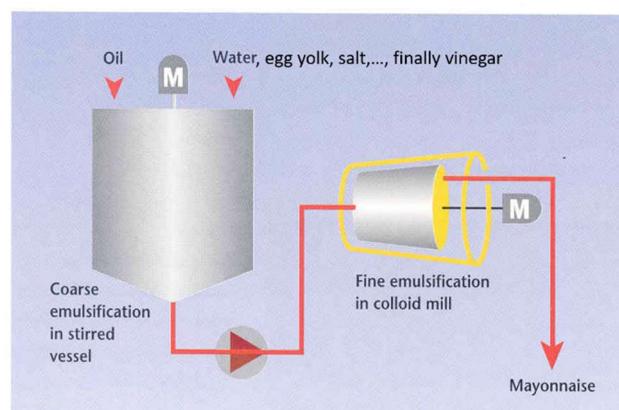
Figure 1 Schematic representation of mayonnaise production.

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