ReDrop: Single-Drop Based Modelling of Extraction

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Separation of individual components from complex mixtures is a challenging task that can be efficiently solved by extraction. Extractor design is challenging as well, as trace impurities strongly influence drop coalescence and thus drop size in the extraction system, which in turn affects drop sedimentation, residence time and ultimately mass-transfer efficiency. To overcome this challenge, pilot-plant experiments are usually conducted, which are expensive and require large quantities of all phases, which are typically not available in the early stages of process development.

An alternative approach to address these issues is droplet-based simulation of extractor performance. Tools have been developed based on the ReDrop concept (Representative Drops), where a sufficiently large number of drops are traced in the equipment, considering the various drop effects that occur, such as sedimentation, coalescence and splitting, chemical reactions, and mass transfer. The model parameters that determine drop behavior, in addition to physical properties, are determined using small quantities of the original material system in standardized cells on laboratory scale. With such simulations, which consider many details of the specific equipment in the drop models, not only process design but also equipment design is possible, i.e. optimizing the geometry of internals and operating parameters for the best equipment performance. Prediction accuracy is better than 10%, including operating limits such as flooding. How well ReDrop can describe real-world extractor performance has been demonstrated for a variety of applications, including complex material systems.