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Population balance modelling of emulsification processes: parameters identification and uncertainty analysis

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Summary:

Emulsions consist of a liquid dispersed in the form of small droplets in an immiscible liquid, usually with the presence of surfactants to stabilize the droplets. They are commonly employed in our daily life like food, cosmetic and pharmaceutical products, but also as intermediate steps in a number of chemical processes[1]. Different emulsification processes exist. Impellers and rotor-stators are employed in batch processes, while static mixers and membranes offer the advantage of being employed in continuous processes. An important characteristic of emulsions is the droplet size distribution (DSD) of the dispersed phase which impacts the emulsion properties (e.g. texture in food), mass surface (e.g. in extraction processes) and stability[2]. During an emulsification process, the dispersed phase undergoes breakage and coalescence phenomena as a consequence of the continuous phase stresses on one side and the surface and viscosity forces of the droplets on the other side. It is now known that the population balance model (PBM) is the best choice for modelling the evolution of the size distribution in these systems. The PBM framework is adapted to track other properties (e.g. chemical composition, shape in crystals), and the variation of the number of entities (here droplets) in the space (e.g. creaming, sedimentation)[3,4].

The physical phenomena occurring during the emulsification process are modelled using kernels describing the frequency of disruption of the droplets, the daughter size distribution (giving the repartition of the volume of a droplet when it breaks up) and the probability of coalescence based on the frequency of droplets collision. A number of breakage and coalescence mechanisms are proposed in literature[5,6]. These kernels rely on empirical parameters that need to be identified. But, it is yet not possible to find in literature a unique set of model parameters (even with the same mechanism functions and in the same conditions) valid for a large domain. This limits the predictive capabilities of the developed models.

Different reasons may explain the discrepancies of the identified parameters in the different studies. First of all, a critical analysis of the related literature reveals that in most cases only partial experimental investigations are reported and used for the validation of the PBE-based models. Even though this is inherent to technical difficulties, the consequences on the reliability of the proposed models outside the investigated domain is questionable. Moreover, emulsification is usually studied in stirred vessels but the non-uniformity of the vessel (mainly in terms of energy dissipation) is usually not considered in the development of the kernels and the identification of their parameters. Also, some works only used the mean diameter of droplets/bubbles for parameter identification, which removes a big part of the information available in the droplet size distribution.

This project aims at proposing a unified approach for uncertainty and sensitivity analysis of PBMs of liquid-liquid dispersions. It constitutes a logic continuity of the works done in our research group in the recent years regarding the modelling of different emulsification processes[7,8]. Emulsification will be investigated in different devices: stirred vessels using impellers or rotor-stators, and static mixers. The advantage of static mixers is that they offer the possibility to have a more uniform energy dissipation than stirred vessels. The advantage of the stirred tank is that lower energy dissipation can be implemented. Thus, using both devices allows us to have a wide variation of energy dissipation. The properties of both liquids will also be investigated, mainly the viscosity of both phases and the fraction of the dispersed phase. Some phenomena may be negligible under certain conditions (e.g. negligible droplet coagulation in diluted conditions, or negligible effect of the droplet viscosity if it is not viscous). Therefore, the identification will be accompanied by a critical sensitivity analysis to ensure good parameter identification and to highlight the ranges of validity. The validity of the available kernels under the different operating conditions will also be investigated.

References

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