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Population balance modeling for the description of mass transfer and chemical reactions in liquid-liquid dispersions

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Highlights

- One- and multi-dimensional population balances are used to model liquid-liquid dispersions.
- The error made with the one-dimensional population balance is quantified.
- Time scales analysis identifies a-priori the type of population balance to adopt.

1. Introduction

The evaluation of the mass transfer rates in turbulent liquid-liquid systems has been historically carried out based on the common assumption that all the dispersed droplets have the same size and chemical composition. This assumption often leads to a wrong description of the physical reality: in fact the droplets may have different size and composition due to the complex interaction between droplet coalescence, breakage, mass transfer and chemical reactions occurring in such systems. The evolution in space and time of each droplet is the result of the interplay between mass, momentum and heat exchange between the phases, and its prediction requires a detailed methodology capable of properly addressing a similar complexity. In this sense, a very powerful tool is Population Balance Modeling (PBM) that can provide a local deterministic description of the joint droplet size-composition distribution. However, such detailed model may be not always needed: when coalescence and breakage dominate, only the size distribution has to be accounted for, whereas on the contrary, when mass transfer dominates the process, very often the joint size-composition distribution must be considered. In this work, a strategy based on the time scale analysis to evaluate a-priori the complexity of the needed model is shown and applied on a realistic test case. The methods here used to efficiently solve the resulting population balance equations are the so-called Quadrature-Based Moment Methods (QBMM) [1].

2. Methods

A population constituted by dispersed droplets in a continuous phase can be formally described in terms of number density function (NDF), representing the number of expected droplets in a certain infinitesimal portion of the physical space within an infinitesimal range of size and composition, and its evolution in space and time can be evaluated through the solution of the so-called Population Balance Equation (PBE) [1]. Two possibilities are available for the PBM. In the simpler approach, a one-dimensional population balance with only droplet size as internal coordinate can be solved. Alternatively, the possibility that droplets of the same size may have had different histories and, consequently, different compositions can be considered through the solution of a multi-dimensional population balance. The multi-dimensional PBM completely describes the whole mass transfer process through the joint droplet size-composition distribution, whereas the one-dimensional PBM assumes that all the droplets have the same composition, introducing a simplification that in some cases might not be acceptable. In this work, a direct quantification of the error made when using the one-dimensional PBM (instead of a multi-dimensional PBM) for a liquid-liquid dispersion undergoing simultaneous coalescence, breakage, mass transfer and chemical reaction. This analysis is carried out for a well-stirred liquid-liquid system. As a first simplification, only one chemical component transfers from the disperse to the continuous phase, where it reacts under isothermal conditions. Water for the continuous phase, octanol for the disperse, benzo[A]pyrene for the transferring component are used as a test case, but the conclusions derived from the present analysis are general and can be applied to other systems [2]. Mixing is here assumed to be fast compared to the other phenomena involved, therefore the system is considered spatially homogeneous with a spatially zero-dimensional model [3].

Through a proper definition of characteristic quantities associated with the investigated system, such as a characteristic total droplet number density and a characteristic concentration of the component transferring from one phase to the other, it is possible to make the governing equations dimensionless and characteristic time scales arise. These time scales are in turn used to identify the controlling phenomenon and the corresponding modeling approach needed.

3. Results and discussion

Fig. 1 reports the results of the analysis for a global volume of α=0.001 as an example. The picture on the left maps the ratio between two time scales by varying two model parameters, the turbulent dissipation rate ε and the kinetic constant of a first order reaction rate that consumes the transferring chemical species. The first time scale corresponds to the overall process considering coalescence and breakage as two processes in parallel, whereas the second time scale is the summation between the time scale for mass transfer and chemical reaction, two phenomena that occur in series. This map can be drawn before running any detailed simulation, as the time scales can be easily evaluated from the models for droplet coalescence, breakage, mass transfer and chemical reaction.

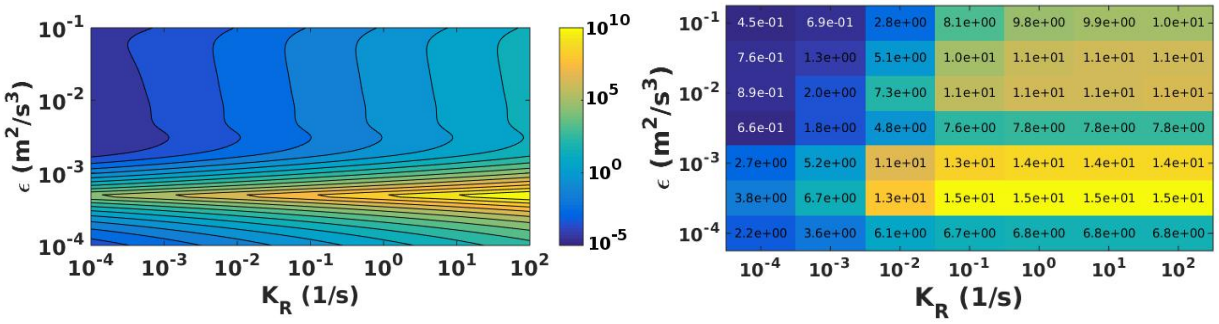

Figure 1. Left: ratio of the overall time scale for breakage and coalescence and the summation of the mass transfer and chemical reaction time scales (in decimal logarithmic scale). Right: Percent error associated with the replacement of the multi-dimensional PBM with the one-dimensional PBM.

The picture on the right show the error in the evaluation of the mass transfer rates when the one-dimensional PBM is used instead of the more detailed multi-dimensional PBM model. As it is possible to observe from the picture, the error is higher when mass transfer and chemical reaction are faster than coalescence and breakage. Based on the obtained results a criterion is established: when the time scales ratio is under 10^2, the error in mass transfer calculation is always below 1% and therefore a one-dimensional PBM can be used.

4. Conclusions

The results shown that when coalescence and breakage prevail, the population of droplets has a more homogeneous concentration of the transferring component within the droplets, whereas when mass transfer and chemical reaction prevail, droplets of the same size may have different composition. In the first case a one-dimensional PBM can be used to estimate the specific surface area, and a single mass balance can be used to calculate the concentration of the transferring component within the droplets. In the second case, mass transfer needs to be described by means of the joint droplet size-composition distribution, which gives a proper expression for both the specific surface area and the driving force of the mass transfer.

References

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Keywords
Liquid–liquid dispersions; Population Balance Modeling; Quadrature-Based Moment Methods; Mass transfer.