ReDrop: single-drop-based modelling of extraction columns

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Introduction

The ReDrop (representative drops) algorithm is a powerful tool that allows to model the behavior of extraction columns of different configurations based on drops modelling. The simulation approach relies on simulating the behavior of a large number of drops along their trajectory through the column. It is based on the experimental and modelling studies on the scale of drops. The different phenomena that can occur to each drop and which are modelled include sedimentation, mass transfer, chemical reactions, coalescence, breakage, swarm effects, axial dispersion, etc. Each of these phenomena is influenced by the geometry of the column and the internals. ReDrop has the advantage to allow the design of large-scale columns of any column type based solely on generic lab-scale single-drop experiments. These lab-scale experiments are standardized and require only some few litres of both phases. This is a significant benefit as compared to the classical design method, which relies on pilot-plant experiments, which require a large amount of the solutions and significant experimental time.

Algorithm

A graphical representation of the ReDrop algorithm is presented in Figure 1. Once the initial parameters are defined, the behaviour of each drop is simulated, regarding all phenomena that can occur. The drops leaving the studied column section are then considered and several parameters are updated accordingly like the continuous-phase concentration. Also, chemical reactions in the drops, in the continuous phase or at the drop interface can be accounted for. The behaviour of a large number of drops is followed over time, which allows to model the transient evolution of different variables such as concentration profiles in the column. Reaching steady state for physical extraction requires only few minutes of computer time.

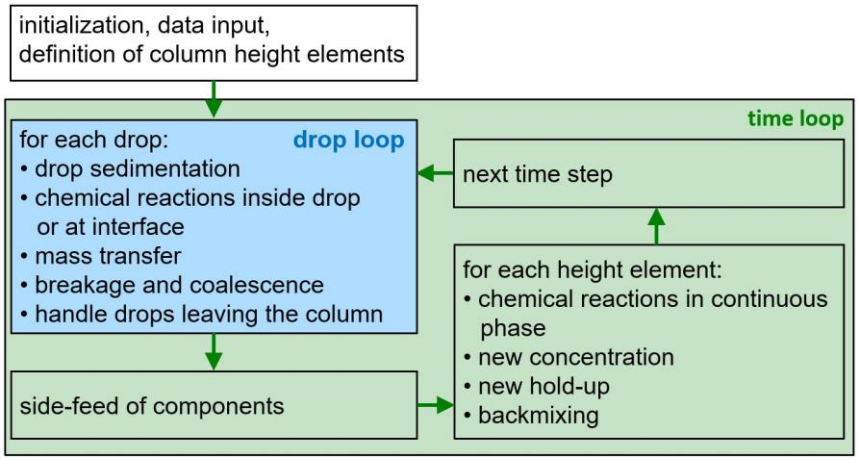

Figure 1: Graphical representation of the ReDrop algorithm.

Applications

ReDrop had been developed and applied to different extraction tasks for more than two decades. Models developed by Henschke allow to describe drop behaviour such as sedimentation velocity, mass

transfer, breakage and coalescence, as well as axial dispersion in the continuous phase (Henschke, 2004). The ReDrop program was then extended over the years. For instance, Kalem (Kalem, 2011) applied the ReDrop algorithm for the modelling of RDC columns with reactive systems and Kalvoda (Kalvoda, 2016) validated a mass-transfer model that accounts for the concentration gradient present in the continuous phase in columns. ReDrop can also predict phenomena such as flooding. In such a case, the flooding is a consequence of the drops' behavior, and not a limit introduced as input to the simulation (Ayesteran, 2015). The ReDrop algorithm can be applied to a wide variety of processes. Material systems used range from the EFCE standard test systems for extraction to systems relevant in biotechnology and ionic liquids (Bednarz, 2019).

Currently ReDrop is extended for the simulation of a new reactive extraction process dedicated to metal recycling in urban mining. Single-drop experiments are conducted to study the reactive extraction of metal ions with different extractants and under varying conditions. A single-drop cell allows to measure the parameters necessary for the mass-transfer and reaction-kinetics model at such conditions. These parameters are then used to model the newly developed process.

Conclusions

ReDrop is thus based on the exact modelling on the droplet scale and predicts the extraction performance on pilot-plant scale. It has been shown that the ReDrop algorithm allows to model the behavior of an extraction column with an accuracy better than 10 % as compared to pilot-scale experiments. The program is flexible as it can be applied to several configurations and material systems with only a few changes in the input files and a defined set of single-drop experiments.

Currently, ReDrop is applied to reactive-extraction processes, where the consistent modelling of the simultaneous processes of mass transfer and reaction kinetics is a challenge. The model, which has been validated on drop level with the help of the single-drop measuring cells, is implemented in ReDrop to allow simulation of a reactive-extraction column. The modelling approach to characterize single-drop reactive behavior will be presented together with how it is embedded in the ReDrop concept.

References:

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