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## Introduction

Conventionally, extraction columns are designed based on pilot-plant experiments. This requires at least several 100 liters of substance of each phase. The scale-up based on pilot-plant experiments is thus expensive while limited in scope. In recent years a design method has been proposed and validated, which is based on drop-based column simulation. This method allows prediction of column performance based on lab-scale experiments with a small amount of original

material system. The results of the single-drop experiments are utilized to fit model parameters of corresponding models describing sedimentation, mass transfer, as well as coalescence and splitting, which are then used in the extraction-column simulation. This simulation method has been implemented based on a Monte-Carlo approach to solve the population balances by regarding a suitably large ensemble of individual drops as they pass through the column [1,2,3,4]. The accuracy obtained up to and including the flooding point is typically better than 10%.

## The ReDrop Concept

With the ReDrop (REpresentative DROPS) program drop population balances are solved as characterized schematically in Figures 1 and 2. A number of drops, typically 1000 per meter of column height, is followed on their trajectories along the column to simulate the transient behavior of an extraction column. For each drop the drop effects are accounted for by appropriate models. The models account for sedimentation, mass transfer, splitting and coalescence, describing also the interactions among the drops and with the internals. Since the material-specific parameters of these models are fitted to experiments of exactly the corresponding drop effect, a good reliability of the final column simulation is achieved.

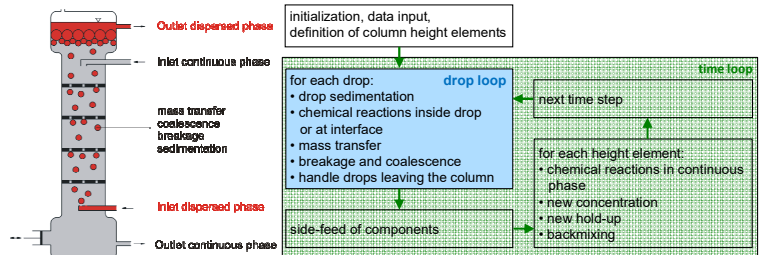


Figure 1. Extraction column

Figure 2. Schematic drop-based ReDrop algorithm

## Different Mass-Transfer Cells

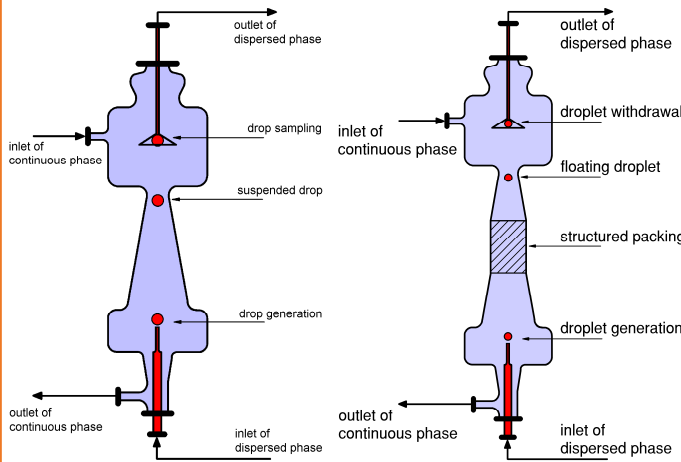


Figure 3. A small mass-transfer cell without internals, to which a small sieve tray can be fitted. The drops are levitated in the conical part for a defined contact time before they are withdrawn and analysed.

Figure 4. A larger cell with a cylindrical section to which regular packings of 40 mm diameter can be fitted. It has been validated that without internals the results are identical to those obtained with the cell shown in Figure 3.

Figure 5. Cell with rotating internals, which allows to evaluate the residence time of drops in different zones, i.e. below, at, and above stirrer zone, together with the corresponding transition probabilities. A drop selection glass sphere has been invented to exclude broken drops from analysis.

Figure 6. In extraction columns drops pass through a concentration gradient, which is not realized in the other cells. So in this cell a dedicated gradient can be imposed and its effect on mass transfer analysed.

## Results

In the different publications cited below, the following results have been obtained for mass transfer:

- mass transfer depends on drop size and velocity
- mass-transfer induced turbulence strongly enhances mass transfer, characterized by the parameter  $C_{prof}$
- in passing a sieve tray, the drop volume is slightly mixed
- for counter sieve trays, the major effect is that the drops are experiencing focused counter-flow of continuous phase significantly enhancing mass transfer during that period, where they cannot pass the holes due to the counterflow.
- packings have hardly an influence on mass transfer, mainly the drop velocity is affected influencing residence time
- only upon first entry to a packing zone mass transfer is slightly enhanced
- also in a stirred Kühni compartment mass transfer is only slightly enhanced
- for several example cases mass transfer in reactive systems could be sufficiently well described with an effective model not regarding the reaction explicitly
- the model description can be improved, if reaction kinetics is accounted for
- linking drop mass transfer to results on reaction kinetics and mass transfer in a Lewis-type cell has not been successful until now
- mass transfer is strongly influenced by a concentration gradient in the continuous phase (see Figure 7), which can be modelled by
  - applying a differential shell model

- modifying the equation above: 
$$D_{d,eff} = D_{phys} + \frac{v_{\infty}}{C_{prof} \left(1 + \frac{\eta_d}{\eta_c}\right)}$$
- allowing enhancement by factor 1.5 due to Marangoni convection, if the concentration gradient at the start exceeds a certain limiting value
- mass transfer in all cases can be characterized with the appropriate model

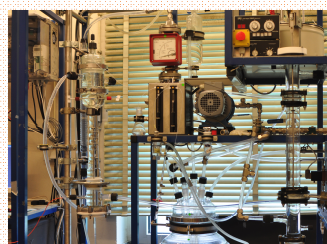


Figure 7. Lab-scale mass-transfer rig

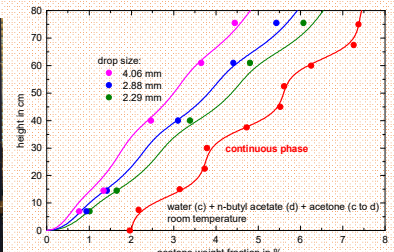


Figure 8. Concentration profiles in gradient cell

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