Single-Drop Experiments for Challenging Conditions as Basis for Extraction-Column Simulations

José Manuel Ayesterán Jerez[1], Florian Buchbender[1], Murat Kalem[2], Eva Kalvoda[3], Andreas Pfennig[4,*].
[1]*AVT - Thermal Process Engineering, RWTH Aachen University, Wüllnerstr. 5, 52062, Aachen, Germany*
[2] *Covestro Deutschland AG, Distillation & Phase Separation, 51365 Leverkusen, Germany*
[3]*TU Graz, Institute of Chemical Engineering and Environmental Technology, Inffeldgasse 25/C/II, 8010 Graz, Austria*
[4]*University of Liège, Department of Chemical Engineering - Product, Environment, and Processes (PEPs), Quartier Agora, Allée du Six Août, 11, 4000 Liège, Belgium*

1. Introduction

In recent years drop-based column simulation has been developed to allow prediction of column performance based on lab-scale experiments with a small amount of original material system. This approach has even proven to be accurate for challenging systems like ionic liquids and industrial systems [1,2]. To increase the accuracy of the simulation, the accuracy and scope of the drop models needs to be extended.

2. Experimental

The goal of a series of studies was to challenge and extend existing drop models. For example in the typical mass-transfer cells a drop is contacted with a continuous phase of constant concentration. In extraction columns this is not observed, the drops instead encounter a continuous phase with a pronounced concentration profile. Also, it has been found in several studies that sedimentation velocity and mass transfer are strongly linked. Thus a single-drop cell has been designed, which allows imposing a concentration profile on the continuous phase through which the drop has to pass for quantifying mass transfer and sedimentation velocity.

The influence of internals on mass transfer needs to be depicted in accurate column simulations. While corresponding cells have already been proposed for sieve trays and packings, the challenges for rotating internals are especially demanding, because chances are high that a drop will be split by interaction with the stirrer or the shear region in its vicinity. To nevertheless be able to attribute an experimental datum to drops of defined diameter, a single-drop cell has been designed, which allows selecting individual drops for the measurement after they passed the internals. For modelling sedimentation in columns with rotating internals the residence times below and above the stirring element together with the corresponding transfer probabilities between these zones have to be characterized experimentally and corresponding models derived.

Reaction kinetics may occur on top of the mass transfer induced by Nernst distribution. This needs to be described by corresponding approaches including reaction kinetics. If suitable models have been found, the results for drops should compare well with those obtained with a defined flat interface, e.g. for experiments performed in a Lewis-type cell.

3. Results and Discussion

With the suitably designed single-drop cells these detailed effects have been investigated. It turns out that conventional models need significant enhancement in order to properly describe the effects addressed, which are encountered in extraction columns under realistic conditions. Besides deriving improved detailed models the insights can be used to optimize extraction-column performance. Thus, a proposal for reducing the volume of stirred columns without significant effect on drop residence times has been derived and experimentally validated.

1) Buchbender, Onink, Meindersma, de Haan, Pfennig, *Chem. Eng. Sci.*, **82,** 167-176 (2012)
2) Buchbender, Schmidt, Steinmetz, Pfennig, *Chem. Ing. Techn*., **84**, 540-546 (2012)

Key words: drop-based modelling, extraction column, single-drop experiments, mass transfer, sedimentation