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# The impact of Marangoni convection on fluid dynamics and mass transfer at deformable single rising droplets – A numerical study

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## Abstract

In this paper, fluid dynamics and mass transfer of single droplets rising in a quiescent ambient liquid are considered. For the first time, full three-dimensional simulations of a deformable droplet dominated by Marangoni convection induced by concentration gradients were performed. A level set based code accounting for the mutual coupling of mass and momentum transfer was developed and implemented in the open-source computational fluid dynamics (CFD) package OpenFOAM<sup>®</sup>. The liquid/liquid extraction test system toluene/acetone/water was investigated, and numerical results were compared with experimental data from literature. The code captures and reproduces the characteristic experimental results: the two step acceleration behaviour, the temporary reduction of the drop rise velocity, and the enhancement of mass transfer depending on the initial solute concentration. The lateral break-out in the drop path at the instant of reacceleration has only been observed experimentally so far. Our simulations reproduce this phenomenon, confirming the existence of pressure gradients across the droplet. Furthermore, our results reveal that the break-out effect is governed by rear vortex detachment.

*Key words:* droplet, Marangoni convection, mass transfer, CFD, level set, extraction

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