### Accepted Manuscript

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PII: DOI: Reference:	S0301-9322(15)00156-1 http://dx.doi.org/10.1016/j.ijmultiphaseflow.2015.06.013 IJMF 2250
To appear in:	International Journal of Multiphase Flow
Received Date:	3 July 2014
Revised Date:	21 June 2015
Accepted Date:	30 June 2015



Please cite this article as: Engberg, R.F., Kenig, E.Y., An investigation of the influence of initial deformation on fluid dynamics of toluene droplets in water, *International Journal of Multiphase Flow* (2015), doi: http://dx.doi.org/ 10.1016/j.ijmultiphaseflow.2015.06.013

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## ACCEPTED MANUSCRIPT

# An investigation of the influence of initial deformation on fluid dynamics of toluene droplets in water

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#### Abstract

The impact of the initial shape on the rise behaviour of single toluene droplets in water was studied numerically. A level set based computational fluid dynamics (CFD) code was implemented in the open-source CFD package OpenFOAM<sup>®</sup>, and fully three-dimensional simulations were performed. Droplets were initialised either as sphere or as ellipsoid, and asymmetries were introduced by rotating the ellipsoid. For the first time, a velocity bifurcation, i.e. the appearance of two different characteristic rise velocities for the same droplet diameter, was reproduced with the simulations, confirming the experimental findings of Wegener et al. (2010). Furthermore, the simulation results illuminate the mechanisms leading to the velocity bifurcation: In contrast to fast droplets, a flow separation is observed for slow droplets, disturbing the internal circulations and increasing both frictional and pressure drag. Moreover, our simulations show velocity oscillations of circulating droplets, which are in agreement with experimental observations of Wegener et al. (2010), and reveal the mechanisms leading to a break-out in the trajectory of these droplets. Finally, the frictional, pressure and total drag coefficients are presented, and their analysis indicates that the variation of the total drag coefficient with the Reynolds number is caused mainly by a change in pressure drag.

*Keywords:* Droplet, Rise velocity, Bifurcation, Drag coefficient, CFD, Level set

Preprint submitted to International Journal of Multiphase Flow

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