**Comparison of numerical approaches for drop breakup in microporous channels**

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**Highlights**

* Comparison of numerical studies. Volume-of-Fluid vs. Lattice-Boltzmann
* Drop breakup is related to interfacial shear stress and pore geometry
* Generic simulations are performed to analyze the breakup processes in complex structures
* Stress related breakup mechanisms enable opportunities in membrane design

**1. Introduction**

Emulsions are widely used in industrial applications. In particular in the food technology and in the pharmaceutical industry the quality of the emulsion is relevant. The membrane emulsification process obtains the advantage to adjust the droplet size distribution according to the pore structure and the geometry of the membrane. The membrane emulsification process is a low stress process which is relevant for the handling of shear sensitive media (i.e. in biological systems). Whereas the emulsification process and influence of the membrane structure and geometry on the final product is well investigated, the liquid deformation and liquid dispersion process inside of the membrane structure is quite unknown. In particular the shear and strain stress at the droplet interface is important, especially in combination with adsorption processes of surfactants. Local stresses determine the droplet deformation and eventually the breakup. On the other hand, shear and strain stresses can influence the adsorbed structures (surfactants) at the interface, in example proteins. In this work numerical investigations with the Volume-of-Fluid-Method were performed to understand stress related breakup mechanisms in microporous structures. Furthermore Lattice-Boltzmann studies were carried out to investigate the effect of non-Newtonian fluid on the breakup process. The results of both methods are complemented to get an overall understanding of the complex breakup mechanisms in membrane emulsification processes.

**2. Methods**

A Volume-of-Fluid method formulation within OpenFOAMS InterFoam solver was implemented. This model enables the calculation of local shear and strain conditions (stress tensor) at the interface of a liquid-liquid system. With this extension the stress residence time behavior at the liquid-liquid interface in idealized pore structures and elementary flow constrictions has been analyzed. The parameters influence on the droplet deformation is carried out and critical shear and strain stresses for droplet breakup are analyzed. The simulation procedure was extended to real membrane pore geometries and compared to the stress conditions and break up mechanisms received from the idealized pore geometries. The inter-particle Shan Chen Lattice Boltzmann model for immiscible fluids is used to analyze the droplet dynamics in porous model structures and real membrane structures. Furthermore, models for shear-thinning and viscoelastic fluids are used to study the differences in the break-up mechanism. Newtonian droplets in non-Newtonian continous phases and vice versa are investigated at different Deborah numbers. Parameters in both numerical studies were varied by the pore geometry, capillary number, contact angle and droplet size.

**3. Results and discussion**

An example of the porous structures investigated and a simulated (VOF) drop within this structure is shown in Fig. 1. For the Volume-of-Fluid Method the results show that liquid-liquid (disperse-continuous) interface stress determines the drop deformation process rather than liquid-solid (disperse-wall) interface stress. The main stress related drop breakup mechanisms were derived. At a critical capillary number the drop detaches from the pore wall based on contact line instabilities, followed by a deformation of the droplet at the liquid-liquid interface due to stress and strain histories, ending up in the breakup of the droplet due to local constrictions. The analysis of local and integral interfacial stress condition gives insight of the geometry and time dependent drop deformation behavior. [1]

The results of the Lattice-Boltzmann studies show that the feedback of the viscoelastic fluid changes the breakup process and thus the resulting drop size distribution. This leads to smaller drop sizes. The local shear rates in the membrane structure induce local shear thinning of the non-Newtonian fluid, which results in a change of the local stress conditions and hence of the drop deformation behavior.



**Figure 1.** CT-scan of a porous membrane structure (a) and a simulated droplet within the membrane structure (b) [1]

**4. Conclusions**

The analysis of the stress dependent drop breakup mechanisms in micro-pores and the investigation of the effect of non-Newtonian fluid on the breakup process enable new opportunities in the design of porous structures to reduce the stress conditions during the emulsification process for the utilization stress sensitive media and for the formulation of certain emulsion properties.

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**References**

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