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# INFLUENCE ON DROPLET FORMATION IN THE PRESENCE OF NANOPARTICLES IN A MICROFLUIDIC T-JUNCTION

by

## *Rui-Jin WANG* and Zhi-Hua LI*

School of Mechanical and Automotive Engineering, Zhejiang University
of Science and Technology, Hangzhou, China

*The droplet formation in the presence of nanoparticles was studied in a T-shaped microfluidic device numerically. Nanoparticles in continuous phase did not influence droplet formation dynamics obviously. Contrarily, the presence of nanoparticles in dispersed phase will influence evidently droplet formation dynamics, the possible reason is that the accumulation of nanoparticles at the liquid-liquid interface would cause the variation of interfacial tension and the anisotropy of nanoparticles' movement at interface. Discussions on microscopic mechanism of droplet formation in the presence of nanoparticles were carried out.*

Key words: *droplet formation, nanoparticles, T-junction*

## Introduction

Over the past decade droplet-based microfluidics has been widely used in the areas of nanomaterials preparation, pharmaceutical analysis, protein engineering, and so on [1-6]. Research works on dynamics behavior of droplet mainly focus on mechanism of droplet formation, control of droplet size. In T-junction microchannels, the dispersed phase liquid is discretized into separate elements by immiscible continuous phase liquid. This process involves complex mechanism, which derives from the force competition among the interfacial tension, viscous shearing, pressure drop, and possible force perturbations out of the system [7-10]. Current computational fluid dynamics (CFD) study has been proven to be a powerful tool to investigate the pressure and velocity distribution, the commercial CFD software is readily a complement for experimental study. Moreover, lattice Boltzmann method (LBM) was also proven to be a valid tool for predicting droplet creation and deformation at microscale [11-15]. However, it remains unclear, how the nanoparticles in fluid influence the droplet formation mechanism and droplet size so far. We intend to investigate the hydrodynamics behavior of droplets containing nanoparticles in this paper numerically.

## Calculation model

The microchannel under investigation is presented in fig. 1 The channel depth is 30 μm. The inlet 1 and inlet 2 are injected with deionized water as continuous phase and silicone oil as dispersed phase, respectively. At wall hydrophobic contact angle is 105°. The inlet
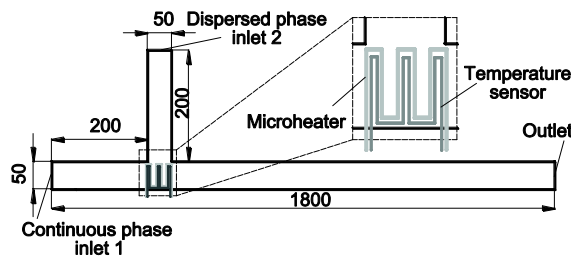
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* Corresponding author; e-mail: wrj5188@163.com

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**Figure 1. Schematic diagram of geometric models**

for dispersed fluid and the main channel for continuous fluid are pre-filled with continuous phase. At the T-junction microheater and temperatue sensors are hypothetically embedded to control and measure the local temperature. The settings of based fluids properties: the viscosity, density, specific heat and thermal conductivity of fluid are 1.003 g/m·s, 0.9982 g/cm$^3$, 4180 J/kgK, and 0.6 W/mK, respectively; the viscosity, density, specific heat, and thermal conductivity of dispersed phase are 50 g/m·s, 0.950 g/cm$^3$, 1630 J/kgK, and 0.16 W/mK, respectively. Density and specific heat of $Fe_3O_4$ nanoparticle are 5.18 g/cm$^3$ and 937 J/kgK. The interfacial tension between deionized water and silicone oil is 30 mN/m at 25 °C. The source term in N-S equation correlated with interfacial tension based on the continuum surface force model can be calculated as described in [5]. Moreover, the nanoparticle continuity and energy equations are derived from Buongiorno [16]. In our simulation, the nanofluid is treated as a single phase, and is considered to be a dilute mixture. Brownian diffusion and thermophoresis, can be regarded as the only slip mechanisms for nanoparticle transport at low Reynolds number in microflow. They are incorporated into the nanoparticle transport equation.

**Results and discussion**

The problem can be described in terms of following dimensional and physical parameters: interfacial tension $\sigma$, channel depth $h$, channel width $w_c$, $w_d$, flow velocity $v_c$, $v_d$, , viscosity $\mu_c$, $\mu_d$, density $\rho_c$, $\rho_d$, (subscript $c$ and $d$ denote that of continuous phase and dispersed phase ). We can define six independent dimensionless parameters based on the abovementioned parameters, $Q = v_d v_d / v_c v_c$, $Ca = \mu_c v_c / \sigma$, $Re = \rho w_c v_c / \mu_c$, $\lambda = \mu_d / \mu_c$, $\Lambda = w_d / w_c$, and $\Gamma = h / w_c$. The droplet diameter $D_d$ is defined as droplet volume divided by channel width of continuous phase, channel width of dispersed phase and depth, *i. e.* $D_d = V_d / w_c w_c h$, here, $V_d$ is droplet volume, which can be exported after calculation, because most of the droplets in published experiments are longer than the width of continuous phase channel. The inlet velocity of continuous phase is set to be 0.12-1.2 mm/s, and the flow rate ratio $Q$ ranges from 0.005 to 5. The capillary number $Ca$ is 0.004-0.04, the Reynolds number Re is about 0.006-0.06, the ratio of depth to width $\Gamma$ is 0.6, channel width ratio $\Lambda$ is 1. The viscosity ratio $\lambda$ is about 50 irrespective of nanoparticles suspending in based fluid. The particle volume fraction of the continuous phase is 0.2%, and that of the dispersed phase is from 0.1% to 2%.

The problem is solved using one set of continuity equations for the entire domain both inside and outside the droplets. Both continuous phase and dispersed are treated as incompressible with no external body forces as the influence of gravity can be regarded as negligible. This is justified by the fact that the Bond number ($Bo = \rho_c g w_c^2 / \sigma$) is well below unity.

Numerical simulations have been performed on the influence of droplet size of nanoparticle volume fraction with various flow rate ratio and capillary number. Theoretically, the viscosity influenced interfacial tension and flow characteristics, and the viscosity of a nanofluid varies with increasing nanoparticle volume fraction. It is a pity, no theoretical model is available for the prediction of the effective viscosity of nanofluids as a function of par-
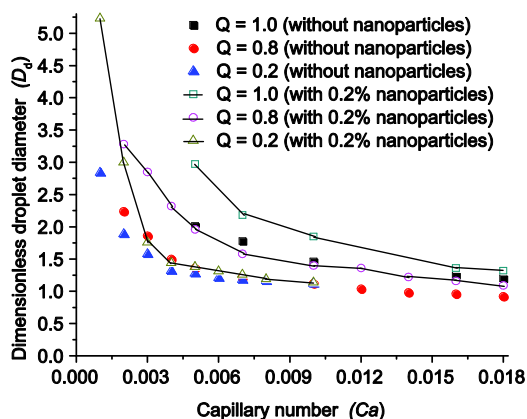
**Figure 2. Effect of 0.2% nanoparticle in the presence of dispersed phase, that of *Ca* and *Q* on the dimensionless droplet diameter at a fixed $\lambda = 50$, $\varLambda = 1$, $\varGamma = 0.6$**
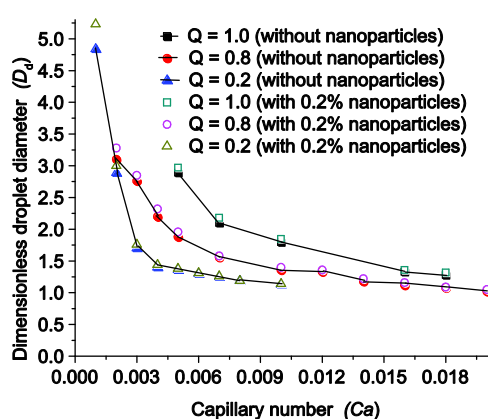
**Figure 3. Effect of 0.2% nanoparticle in the presence of continuous phase, that of *Ca* and *Q* on the dimensionless droplet diameter at a fixed $\lambda = 50$, $\varLambda = 1$, $\varGamma = 0.6$**

ticle volume fraction so far. There are many established results about the effects on the droplet size of capillary number and flow rate ratio in the absent of nanoparticle in fluid [17, 18]. To insight effect of the presence of nanoparticles in dispersed phase, numerical simulations are carried out at a fixed $\lambda = 50$, $\varLambda = 1$, $\varGamma = 0.6$, flow rate ratio *Q* is 1.0, 0.8, 0.2, respectively. Capillary numbers range from 0.001-0.02, for such small values of capillary numbers the droplet formation is in the squeezing (pressure dominated) regime, suggesting that interfacial tension dominates viscous stress. We can see from fig. 2., nanoparticles in dispersed phase affect the droplet size obviously, especially at low *Ca* and *Q*, nearly 50% reduction can be achieved.

The reasons should be that, nanoparticles increase slightly the effective viscosity on the one hand, decrease violently the interfacial tension on the other hand. In the microscopic view, Brownian motion and thermophoresis cause nanoparticle enrichment at interface. In addition, Brownian motion is anisotropic, thermal motion of nanoparticle takes place more effortless tangential to interface than that of normal to interface because of the constraint of interfacial tension. However, in the presence of nanoparticles in continuous phase, less than 10% reduction of the droplet size come into being even at very low *Ca* and *Q* (fig. 3), because the variation of viscosity ratio ($\lambda$) is not so great, that only a slightly influence has been exerted on interfacial tension and droplet formation process.

## Conclusions

The droplet formation process of silicone oil containing nanoparticles in deionized water as continuous phase was investigated for different flow conditions, such as capillary number, and flow rate ratio. With thorough parametric studies, we elaborated on the strong effect of interfacial tension on the droplet size in a microfluidic T-junction. We observed that interfacial tension of nanoparticles uniform suspension in silicone oil as dispersed phase strongly affects the droplet formation in low capillary number and Reynolds number microflow, likely reason is that the accumulation of nanoparticles at the liquid-liquid interface would cause the variation of interfacial tension and the anisotropy of particles' movement at interface. The mechanism is very complicated, because the integrated influence of particle

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movement and interaction should be taken into account to estimate effective viscosity and interfacial tension. The Brownian motion and adsorption of nanoparticles at the interfaces were identified as mechanisms for reduced the interfacial tensions of nanofluid. Contrarily, nanoparticles in continuous phase did not influence droplet formation dynamics obviously.

## Acknowledgments

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