SIMULATION OF THE ALCOHOL-OIL MIXTURE IN A T-SHAPED MICROCHANNEL USING THE DISSIPATIVE PARTICLE DYNAMICS METHOD ON GPU DEVICES

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Abstract. *Multiphase fluid motion in microchannnels involves complicated fluid dynamics and is fundamentally important to diverse practical engineering applications. Among several application, the alcohol-oil mixture is particularly important due to its application for biodiesel production. In this work, the mixture of immiscible fluids alcohol-oil in a square T-shaped microchannel was investigated using the Dissipative Particle Dynamics (DPD) method available in the HOOMD simulator, that runs on a single graphic processing unit (GPU). The immiscible fluids were achieved by increasing the repulsive force between species. The fluid properties and hydrodynamic behavior were discussed in function of model parameters. The simulation results agree with data published in the literature showing that the DPD is appropriate for simulation of mass transport on complex geometries in microscale on a single GPU.*

Keywords*: Microchannel, Two Phase Flow, Dissipative Particle Dynamics, GPU, HOOMD-blue.*

1. INTRODUCTION

Currently, there is a growing interest in microfluidic devices as a powerful tool to produce valuable chemicals and overcome some problems found in a variety of industrial fields. Microfluidic devices provide efficient solutions to improve mixing and mass/heat transfer, therefore, enhancing reaction rate and reducing residence time in comparison with conventional process. Today, a wide range of applications, such as cell encapsulation (Hernández et al., 2010), drug delivery (Yang et al., 2011), chemistry analysis (McMullen and Jensen, 2010), micromixer (Falk and Commenge, 2010), microreactors (Yoshida et al., 2011), lab-on-a-chip devices (Fernandes and Ferreira, 2006; Fonseca et al., 2007), among others can be found, for which a number of excellent general reviews (Hessel and Löwe, 2003a,b,c) and books (Ehrfeld et al., 2000, Hessel et al., 2004, 2005) are available in the scientific literature. Among several applications of microfluidic devices, emulsification process carried out by the mixing of two immiscible fluids in microchannels have attracted extensive attentions due to its wide range of applications in the food, pharmaceutical, and cosmetics industry (Anna et al., 2003; Doku et al., 2005), multiphase mixing devices and microreactors (Abou-Hassan et al., 2010), and DNA analysis (Njoroge et al., 2011). Lately, the alcohol-oil mixture has been widely studied due to its application for biodiesel production (Xie et al., 2012). Biodiesel synthesis involves a transesterification reaction between alcohol and oil, thus several aspects have to be considered to enhance the efficiency of the process such as the immiscible characteristics of alcohol and oil phases (Qiu et al., 2010). In capillary reactors, the oil phase and the alcohol phase are separated from each other due to the high interfacial forces between the two phases, resulting in a slug flow and with the transesterification reaction proceeding, the flow pattern does not change at the outlet of microchannel with formation of ester and glycerol phases (Sun et al., 2008). Droplet formation process in a microchannel involves complex mechanism, which is determined by fluids properties (viscosities and surface properties), flow conditions (flow rates and velocity) of the two immiscible fluids and geometry of the microchannel (width and depth) (Li et al., 2012). The various parameters involved mean that optimizing the liquid–liquid multiphase flow in microreactors requires extensive experimental works. Therefore, numerical studies on such phenomena are essential to provide a better understanding of the process.

In recent years, experimental and numerical studies have been performed on flow pattern transitions and mechanisms of droplet formation in the mixing of two immiscible fluids in microchannels. Most of the numerical works for fluid flow simulations in microchannel are based on solving the continuum Navier–Stokes equations using the computational fluid dynamics (CFD). However, simulating complex flows such as multiphase/multicomponent flows has been a challenge to conventional CFD because of the moving and deformable interfaces. The interfaces between different phases (liquid and vapor) or components (e.g, alcohol and oil) originate from the specific interactions among fluid molecules. Therefore it is difficult to implement such microscopic interactions into the macroscopic Navier-Stokes equation. Recently, considerable attention has been given to particle dynamics techniques such as Molecular Dynamics

(MD) (Allen and Tildesley, 1987; Rapaport, 1995), Lattice Boltzmann method (LBM) (Li et al., 2012; Wang et al., 2011; Gong et al., 2010; Wu et al., 2008), Smoothed Particle Hydrodynamics (SPH) (Liu and Liu, 2005), and Dissipative Particle Dynamics (DPD) (Chen et al., 2007; Liu et al., 2007). MD is a fundamental way to understand the behavior of multiphase flow in microchannels, but due to the very small length and time scales associated, this method is computationally expensive and cannot be applied to many practical problems. LBM has been extensively investigated and extended to a wide range of applications such as colloidal systems and multiphase flows. This method has some disadvantages that are associated with the restriction of the dynamics to the streaming of "particles" between adjacent nodes on a regular lattice (Liu et al., 2007). SPH was originally invented to solve astrophysical problems and it has been gradually modified for much smaller scale. The SPH method for mesoscopic applications is still under development, and quantitative relationships between model parameters and the macroscopic properties of the fluids are difficult to establish (Tartakovsky and Meakin, 2005). DPD is a relatively new mesoscale modeling technique that has been used to simulate the behavior of complex fluids. Dissipative particle dynamics (DPD), which was introduced by Hoogergrugge and Koelman (1992), is an effective approach in simulating mesoscale hydrodynamics with its basis in statistical mechanics founded by Español and Warren (1995), and Marsh (1998). In DPD simulations, the particles represent a small cluster of atoms or molecules. In this method, particle size and time step may be much larger than on MD, making it much more efficient for the purpose of simulating macroscopic hydrodynamics. In this method, the particles move off-lattice interacting with each other through a set of prescribed and velocity-dependent forces. DPD method has been successfully extended to many applications including colloidal suspensions, surfactants, dilute polymer solutions, and biological membranes.

To our knowledge, there are few studies about droplet formation process in a microchannel using DPD method on GPU devices. GPU-accelerated implementations of DPD method have proven to be very fast compared to running a simulation on a single CPU core, achieving several orders of magnitude speed-ups (Phillips et al., 2011). In this work, the dissipative particle dynamics (DPD) method available in the HOOMD-blue simulator (Anderson et al., 2008; http://codeblue.umich.edu/hoomd-blue) was used to simulate droplet formation process in the mixing of alcohol-oil immiscible fluids in a three dimensional square T-shaped microchannel on a single GPU device. The immiscible fluids were achieved by increasing the repulsive force between species. The fluid properties and hydrodynamic behavior were discussed in function of model parameters.

2. NUMERICAL METHOD

2.1 Dissipative Particle Dynamics Method (DPD)

In the DPD method, a set of interacting particles is considered and Newton's second law governs the motion of each particle. For simplicity, it is assumed that all particles have unity masses. The equation of motion for particle *i* can therefore be expressed as:

$$\frac{dr_i}{dt} = v_i \tag{1}$$

$$\frac{dv_i}{dt} = f_i = f_i^{int} + f_i^{ext} \tag{2}$$

where $\mathbf{r}_i$ and $\mathbf{v}_i$ are the position and velocity vectors, and $\mathbf{f}_i^{ext}$ is the external force including the effects of gravity. The pairwise additive interparticle force acting on particle *i*, $\mathbf{f}_i^{int}$, consists of a conservative force, $\mathbf{F}^C_{ij}$; a dissipative force, $\mathbf{F}^D_{ij}$; and a random force, $\mathbf{F}^R_{ij}$:

$$f_i^{\text{int}} = \sum_{j \neq i} F_{ij} = \sum_{j \neq i} F_{ij}^C + F_{ij}^D + F_{ij}^R \tag{3}$$

where $\mathbf{F}_{ij}$ is the force on particle *i* due to interaction with particle *j*, which is equal to $\mathbf{F}_{ji}$ in magnitude and opposite in direction. Momentum is rigorously conserved due to the symmetry of the interaction forces, $\mathbf{F}_{ij}=-\mathbf{F}_{ji}$. The pairwise particle-particle interactions have a finite cutoff distance, r_c, which is usually taken as the unit of length. The conservative force, $\mathbf{F}^C_{ij}$, a soft interaction acting along the line of particle centers, is often given the form:

$$F_{ij}^C = a_{ij}\, w^C(r)\, \hat{r}_{ij} \tag{4}$$

where a_{ij} is the maximum repulsion between particle *i* and particle *j*; and $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, $r=r_{ij}=|\mathbf{r}_{ij}|$, and $\hat{\mathbf{r}}_{ij}=\mathbf{r}_{ij}/r_{ij}$. $w^C(r_{ij})$ is the weight function for the conservative force, and is usually selected as:

$$w^C(r)=\begin{cases}(1-r) & r<1.0\\ 0 & r\geq 1.0\end{cases} \tag{5}$$

The dissipative force, $\mathbf{F}^D_{ij}$, is given by:

$$F^D_{ij}=-\gamma\ w^D(r_{ij})\left(\hat{r}_{ij}\cdot v_{ij}\right)\hat{r}_{ij} \tag{6}$$

where γ is a coefficient, $\mathbf{v}_{ij}=\mathbf{v}_i-\mathbf{v}_j$, and $w^D(r_{ij})$ is a distance-dependent weight function. The random force $\mathbf{F}^R_{ij}$ is also dependent on the relative positions of the particles as:

$$F^R_{ij}=\sigma\ w^R(r_{ij})\ \xi_{ij}\hat{r}_{ij} \tag{7}$$

where σ is a coefficient, $w^R(r_{ij})$ is a distance-dependent weight function, and ξ_{ij} is a random variable with a Gaussian distribution and unit variance. The dissipative force and random force also act along the line of particle centers and therefore also conserve linear and angular momentum. In order to recover the proper thermodynamic equilibrium for a DPD fluid at a prescribed temperature T, the coefficients, γ and σ, and the weight functions, $w^D(r_{ij})$ and $w^R(r_{ij})$, for the random force and the dissipative force are related by:

$$w^D(r)=\left[w^R(r)\right]^2 \tag{8}$$

$$\gamma=\frac{\sigma^2}{2k_BT} \tag{9}$$

as required by the fluctuation-dissipation theorem. In Eq. (9), k_B is the Boltzmann constant. All of the interaction energies are expressed in units of k_BT, which is assigned a value of unity. One simple and commonly used choice is:

$$w^D(r)=\left[w^R(r)\right]^2=\begin{cases}(1-r)^2 & r<1\\ 0 & r\geq 1\end{cases} \tag{10}$$

The random fluctuation force, $\mathbf{F}^R_{ij}$, represents the effects of thermal fluctuations and acts to heat up the system. The dissipative force, $\mathbf{F}^D_{ij}$, represents the effects of viscosity and acts to reduce the relative velocity of the particles, thus removing kinetic energy and cooling down the system. Consequently, the fluctuating and dissipative forces act together to maintain an essentially constant temperature with small fluctuations about the nominal temperature T. Dissipative particle dynamics simulations are essentially thermostatted molecular dynamics simulations with soft particle-particle interactions (Liu et al., 2007).

2.2 Microfluidic Device Simulation

2.2.1 Geometric Model

The most popular microfluidic device used for mixture immiscible fluids is the T-shaped junction (Fig. 1). In this geometry two microchannels merge at a right angle. The main channel carries the continuous fluid (alcohol-phase) and the lateral channel supplies the fluid that will be dispersed (oil-phase) (Fig. 1a). In the DPD model, the microchannels have rectangular cross-sections and the size of the main and lateral channel is $-22 \leq x \leq -16$, $-3 \leq y \leq 3$, $-25 \leq z \leq 25$ and $-16 \leq x \leq 25$, $-3 \leq y \leq 3$, $-3 \leq z \leq 3$, respectively. In this simulation, the initial configuration of fluids and wall particles were generated separately. Initially, the DPD particles were randomly injected into a computational domain and after equilibration, the particles around of the boundaries were frozen and became the stationary wall particles. Therefore, the walls of the microchannels were represented by particles that have a disordered internal structure. Subsequently, the fluid particles were then randomly injected into the channel. The fluid particles representing the alcohol-phase were injected in the main channel of the domain (blue particles in the Fig. 1b) and particles representing the oil-phase were introduced in the lateral channel (yellow particles in the Fig 1b). The surface tension of the fluids is determined by the interplay between the attractive and repulsive components of the interaction between the fluid particles. In addition, the interaction between the wall particles and the fluid particles was setted to give adequate wetting behavior and capillary forces. Periodic boundary conditions (http://codeblue.umich.edu/hoomd-blue) were applied in Z-direction of fluids inlet.

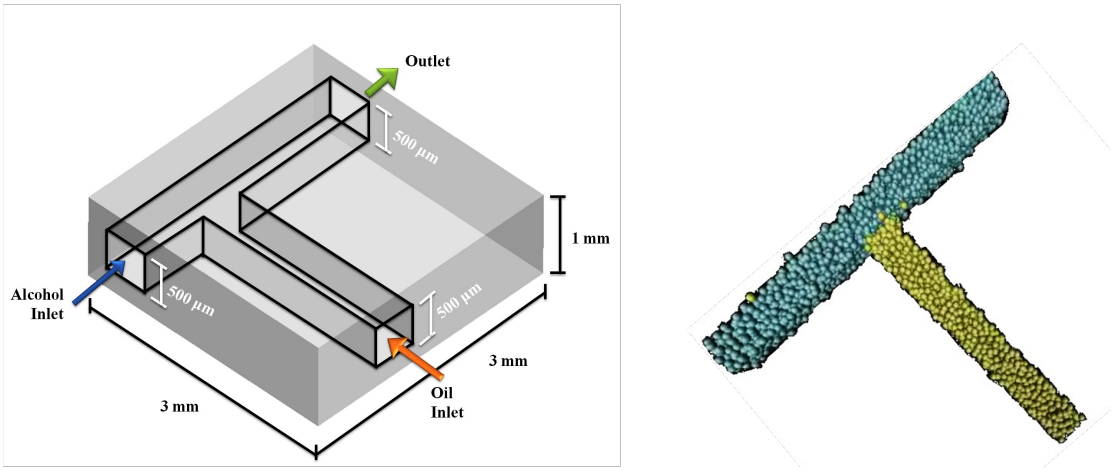


Figure 1. The modeling domain of the T-shaped microchannel: (a) Schematic representation of T-shaped microchannel; (b) Representation using DPD method: blue particles represent the alcohol-phase and yellow particles represent the oil-phase.

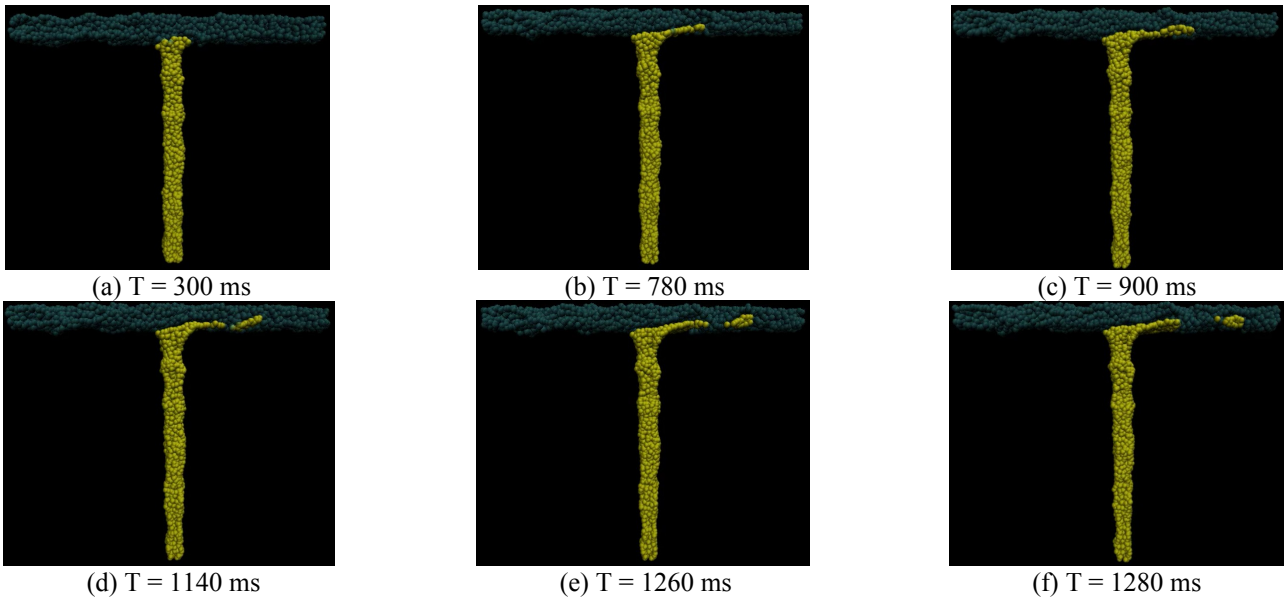
2.2.2 Setting-Up Boundary Conditions

To simulate injection of fluid into the microchannel, the periodic boundary condition was used along the z direction in the main microchannel, and no-slip boundary conditions were applied on the channel walls. The coefficient used in the DPD model was γ=1.5. The time step, Δt, in the time integration algorithm were taken as 0.001. In DPD model, the interfacial tension and wettability between the solid walls (particles A) and alcohol (particles B) and oil (particles C) fluids interfaces are governed entirely by unlike parameters a_{AB}, a_{AC} and a_{BC}, therefore, the parameters for the interaction were A=100, $r_{c,A}$=1.0, B=25, $r_{c,B}$=2.0 and C=15, $r_{c,C}$=2.0. A total of 62500 DPD particles were used, in which 3263 fluid particles were placed in the microchannels and 59237 wall particles are located in the microchannels walls.

3. RESULTS AND DISCUSSION

3.1 Square Microchannel Flows of Immiscible Fluids

T-shaped microchannels are important components in microfluific devices and simulating the multiphase fluid dynamics in microchannnels is essential to the understanding of dynamic physics in microfluidic devices. In this section, are presented the results of alcohol-oil multiphase flow using the DPD model described in previous section (2.2 Microfluidic Device Simulation) and comparable to experimental and theoretical results published in the literature. Figure 2 shows the sequential snapshots of the fluid motion in the T-shaped microchannel obtained using the DPD model. The oil particle (yellow) were pushed in the alcohol particles flow (blue) and formed a drop. This is the expected behavior. Future works include the fine tunning of the simulation model parameters such that the simulation fits more precisely the experimental results, and the simulation of this same problem on a custom simulator that is being developed by Prof. Ferreira's group. The custom simulator is beind developed to run on a cluster of GPUs, so that larger problems may be simulated or the same problem may be solved on shorter run times, and more boundaries conditions, like constant force, are being included on the code to easy the simulation of real devices like this microfluidic mixers.



(a) T = 300 ms (b) T = 780 ms (c) T = 900 ms

(d) T = 1140 ms (e) T = 1260 ms (f) T = 1280 ms

Figure 2. Simulation of fluids motion in the T-shaped microchannel using DPD model. The figures (a)-(f) show the DPD simulation snapshots at different times.

3.2 Discussion on Set Parameters in the DPD Model

In general there is no simple relation between the macroscopic fluid properties and the parameters of the DPD model. Therefore, the assignment of boundary conditions is not a simple task.

4. CONCLUSIONS

In this work is presented the simulation of multiphase flow in T-shaped microchannel using a dissipative particle dynamics (DPD) method. The simulation showed that multiphase flow in microchannels is a complex phenomena where several factors interplay such as viscous, capillary and gravitational forces, microchannel geometry, inflow conditions, and fluids properties. The numerical results obtained by using DPD agreed well with those from others sources showing that potential of DPD method for modeling multiphase flow in microfluidic devices.

5. ACKNOWLEDGEMENTS

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