ABSTRACT

In this work, the effect of applying an electric field on droplet formation in a T-junction microfluidic device is examined by simulations based on a recent technique known as lattice Boltzmann method (LBM). The electric field is applied in the main channel just beyond the confluence of the continuous and dispersed phases. A combined electrohydrodynamics-multiphase model that can simulate the flow of immiscible fluids in the presence of an electric field is developed and validated. The same model is then applied to study the droplet formation process in a T-junction microfluidic device at a capillary number of 0.01 and at different dispersed to continuous phase flow rate ratios. Results show that there is a decrease in the droplet size and an increase in formation frequency as the electric field is increased. The interplay of the electric and interfacial forces on droplet formation is investigated.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$B$</td>
<td>droplet length perpendicular to electric field direction</td>
</tr>
<tr>
<td>$C$</td>
<td>color function</td>
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<tr>
<td>$Ca$</td>
<td>capillary number</td>
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<tr>
<td>$D$</td>
<td>droplet deformation</td>
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<tr>
<td>$d$</td>
<td>discriminating function</td>
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<tr>
<td>$E$</td>
<td>electric field</td>
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<tr>
<td>$e_i$</td>
<td>lattice speed of particles moving in direction $i$</td>
</tr>
<tr>
<td>$F$</td>
<td>force</td>
</tr>
<tr>
<td>$L$</td>
<td>droplet length along electric field direction</td>
</tr>
<tr>
<td>$n$</td>
<td>normal vector at the interface</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure</td>
</tr>
<tr>
<td>$Q$</td>
<td>flow rate ratio - dispersed to continuous phase</td>
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<tr>
<td>$q$</td>
<td>volume charge density</td>
</tr>
<tr>
<td>$R$</td>
<td>inner to outer fluid conductivity ratio</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$r_o$</td>
<td>initial radius of the droplet</td>
</tr>
<tr>
<td>$S$</td>
<td>inner to outer fluid permittivity ratio</td>
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<tr>
<td>$U$</td>
<td>electric potential</td>
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<tr>
<td>$u$</td>
<td>velocity</td>
</tr>
<tr>
<td>$w_i$</td>
<td>lattice weights</td>
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Greek Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>$\tau$</td>
<td>relaxation time</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>gradient</td>
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<tr>
<td>$\gamma$</td>
<td>interfacial tension</td>
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$^1$ Corresponding author
\[ \rho \text{ density} \]
\[ \beta \text{ parameter controlling the width of the interface} \]
\[ \kappa \text{ curvature} \]
\[ \varepsilon \text{ permittivity} \]
\[ \sigma \text{ conductivity} \]
\[ \mu \text{ dynamic viscosity} \]
\[ \nu \text{ kinematic viscosity} \]
\[ \Phi \text{ source term} \]

**Subscripts**
- B blue fluid
- R red fluid
- i index
- c continuous phase
- d dispersed phase

**INTRODUCTION**

The area of droplet-based microfluidics has emerged out of the need to overcome the shortcomings of continuous-flow microfluidics such as contamination due to diffusion, surface adsorption [1] and dispersion, which lead to varying reaction times affecting throughput of microfluidic devices [2]. These effects become more prominent as the size of the microfluidic device is decreased. Droplets provide an ideal platform for isolating the species within and dealing with very small amounts of reagents, thereby opening huge opportunities in drug discovery and biology. The size of droplets formed in microfluidic channels is affected by the flow rates and properties of the two immiscible fluids used and geometry of the microchannel. If these parameters are fixed, it is difficult to exercise control over the size and frequency of formation of the droplets. One of the ways to secure greater flexibility over droplet parameters is by setting up an electric field in the microchannel.

Electrohydrodynamics (EHD) is the study of fluid motion in the presence of an external electric field. Depending upon the physical properties of the fluid like conductivity and permittivity, a droplet can get deformed into different shapes in the presence of an electric field. For static fluid, if a droplet acts as a perfect insulator or is more conductive than the surrounding fluid, it gets deformed into prolate shape. In some experimental results, oblate shape of droplets was also noted and to support those results, Taylor proposed the leaky dielectric model [3, 4, 5]. According to this model, both the droplet and the surrounding fluids are considered to have finite conductivities and when an electric field is applied, charge gets accumulated at the droplet interface. Due to this charge, tangential stresses are generated on the surface of the droplet resulting in an oblate shape. Many theoretical and experimental studies have been carried out to determine the effect of an electric field on two-fluid systems [6, 7, 8]. Fernandez et al. [9] used the finite volume method to study the effect of electrostatic forces on the distribution of droplets in a channel flow. Zhang and Kwok [10] analyzed the change in the shape of 2D droplets in the presence of electric field using the lattice Boltzmann method (LBM). Tomar et al. [11] studied droplet deformation using volume-of-fluids approach. All these studies have used leaky dielectric model for simulating the effect of electric field on the droplet.

In this paper, the leaky dielectric model is used and simulations are performed using the lattice Boltzmann method. LBM is an attractive alternative to conventional computational fluid dynamics to simulate multicomponent flows analyzed in this paper as it does not require separate treatment of the interface. Using LBM, we have developed a coupled electrohydrodynamics [12]-multiphase [13, 20] model and the results obtained are validated with the theoretical models. The same model is then applied to study the droplet formation process in a T-junction microfluidic device.

**MODEL DEVELOPMENT**

LBM has been applied to simulate multiphase flow (silicone oil + water) in a T-junction microfluidic channel in the presence of an electric field. At the interface of the two phases, stress boundary condition is imposed by incorporating a source term in the collision step [14]:

\[ f_i(x,t + \delta t) = f_i(x,t) - \frac{(f_i - f_i^{eq})}{\tau_f} + \Phi_i \quad (1) \]

An interfacial force acts normal to the interface with magnitude proportional to the gradient of the phase field

\[ C = \frac{(\rho_R - \rho_B)}{(\rho_R + \rho_B)} \text{ or the color function} \quad (2) \]

The equilibrium distribution \( f_i^{eq} \) in D2Q9 is given by:

\[ f_i^{eq} = w_i \rho [1 + 3e_i \cdot u_i + \frac{9}{2} (e_i \cdot u_i)^2 - \frac{3}{2} u_i \cdot u_i] \quad (3) \]

For the D2Q9 lattice used for simulation, the weights \( w_i \) are given by:

\[ w_i = \begin{cases} 4/9 & ; i = 0 \\ 1/9 & ; 1 \leq i \leq 4 \\ 1/36 & ; 5 \leq i \leq 8 \end{cases} \quad (4) \]

The lattice velocities \( e_i \) in the above equations are given by Eq. (5) and are also shown in Fig. 1.

\[ e_i = \begin{cases} 0 & ; i = 0 \\ \left( \cos \frac{i-1}{2} \pi, \sin \frac{i-1}{2} \pi \right) & ; 1 \leq i \leq 4 \\ \sqrt{2} \left( \cos \frac{2i-9}{4} \pi, \sin \frac{2i-9}{4} \pi \right) & ; 5 \leq i \leq 8 \end{cases} \quad (5) \]
To sharpen the interface, minimize spurious velocities and eliminate lattice-pinning, the post-collision distributions of the two color fluids, red and blue are computed as [14]:

\[ f_{i,R} = \frac{\rho_R}{\rho_R + \rho_B} f_i + w_i \beta \frac{\rho_R \rho_B}{\rho_R + \rho_B} e_i \cdot n \] (6)

\[ f_{i,B} = -\frac{\rho_B}{\rho_R + \rho_B} f_i - w_i \beta \frac{\rho_R \rho_B}{\rho_R + \rho_B} e_i \cdot n \] (7)

where \( \beta \) is the anti-diffusion parameter, with a value of 0.7. This keeps spurious velocities fairly low and maintains a sharp interface between the two phases [20].

Implementation of the leaky dielectric model with diffuse interface

The electric forces experienced by fluid particles can be written in terms of \( E \), the electric field, \( \varepsilon \), the local fluid permittivity and \( q \), the free charge density. Electrostriction forces have been neglected since the fluid is considered to be incompressible.

\[ \mathbf{F}_E = q \mathbf{E} - \frac{1}{2} \mathbf{E}^2 \nabla \varepsilon \] (8)

The first term corresponds to the coulombic force while the second one corresponds to dielectrophoretic force. The free charge density \( q \) is given by:

\[ q = \nabla \cdot (\varepsilon \mathbf{E}) \] (9)

Electric field is given as:

\[ \mathbf{E} = -\nabla U \] (10)

The charge conservation is governed by the electrostatic law:

\[ \nabla \cdot (\sigma \nabla U) = 0 \] (11)

To solve this equation using LBM, particle distributions \( h_i \) are defined such that:

\[ U = \sum_i h_i \] (12)

The evolution of these particles is described by the following equation:

\[ h_i(x, t + \delta t) = h_i(x, t) - \frac{(h_i - h_i^{eq})}{\tau_i} \] (13)

where relaxation time is given as:

\[ \tau_i = 3\sigma + 0.5 \] (14)

and the equilibrium distributions \( h_i^{eq} \) are given as:

\[
\begin{align*}
 h_i^{eq} &= \begin{cases} 
 \frac{4}{9} U & ; \quad i=0 \\
 \frac{1}{9} U & ; \quad 1 \leq i \leq 4 \\
 \frac{1}{36} U & ; \quad 5 \leq i \leq 8
\end{cases}
\end{align*}
\] (15)

To obtain smooth functions for permittivity and conductivity, the mixture properties have been assumed to follow [10]:

\[ \varepsilon = \frac{\varepsilon_R \rho_R + \varepsilon_B \rho_B}{\rho_R + \rho_B} \] (16)

\[ \sigma = \frac{\sigma_R \rho_R + \sigma_B \rho_B}{\rho_R + \rho_B} \] (17)

In the collision step of \( f \) particle distributions, the source terms due to both the interfacial and electric forces are incorporated:

\[ \Phi_i = \Phi_i^{\text{interfacial}} + \Phi_i^{\text{electric}} \] (18)

RESULTS AND DISCUSSION

Model Validation

The validity of the multiphase model has been established by conducting the static droplet test. Two-dimensional simulations were run with the uniform initial pressure throughout a 101 x 101 periodic domain as the initial condition for different initial radii of the bubble. The relation between pressure inside and outside the bubble is given by Laplace’s Law:

\[ p_{in} - p_{out} = \delta p = \frac{\gamma}{r_0} \] (19)
Thus a linear dependence of $\delta p$ with $1/r_o$ will indicate the model correctly incorporates the physics involved at the interface. The same was observed in the present LBM simulations. The plot of $\delta p$ vs. $1/r_o$ obtained from the simulations is shown in Fig. 2.

![Graph showing the relationship between $\delta p$ and $1/r_o$.](image)

**FIGURE 2:** DIFFERENCE IN THE INSIDE AND OUTSIDE PRESSURE $\delta p$ (LB units) FOR STATIC DROPLET TEST WITH $\gamma = 0.01$ FOR DIFFERENT DROPLET RADIUS $r_o$ (LB units). THE LINEAR VARIATION SHOWS A CONSTANT VALUE OF INTERFACIAL TENSION GIVEN BY THE SLOPE OF THE GRAPH.

In the presence of an electric field, the droplet shape changes to either prolate spheroid or oblate spheroid and, for small values, the deformation $D$ is governed by [18]:

$$D \equiv \frac{L - B}{L + B} = \frac{(R^2 + R + 1 - 3S)\varepsilon_m E^2 r_0}{3S(1 + R)^2 \gamma}$$

(20)

The sign of the discriminant $d = R^2 + R + 1 - 3S$ determines the final shape of the drop. To validate the electrohydrodynamic model, droplet deformations obtained using Eq. (20) were compared with those obtained from LBM simulations. These simulations were conducted for a droplet in presence of an electric field on a domain of size 128x128. For fluid particles, periodic boundary conditions were implemented. The non-dimensional density of the two fluids was set to 1.0. A uniform potential was imposed at the right and left boundaries (Fig. 3) and linearly varying potential from the right to left at the top and bottom boundaries. At the boundary nodes, three out of the nine particle distributions $h_i$ will be unknown. These have been calculated using the fact that the sum of particle distributions along opposite directions is equal to the sum of their equilibrium distributions [17]. For example, for the left boundary, the unknown distributions $h_1$, $h_5$ and $h_8$ can be calculated using:

$$h_{i, unknown} = h_{i, opposite}^e + h_i^e - h_{i, opposite}$$

(21)

For $d > 0$, the drop deforms into a prolate spheroid with lengthening of the axis along the electric field and shortening of the axis perpendicular to it. For $d < 0$, the droplet axis perpendicular to the electric field lengths.

![Diagram showing a droplet in the presence of an electric field](image)

**FIGURE 3:** PROLATE SHAPE ATTAINED BY DROP IN THE PRESENCE OF AN ELECTRIC FIELD.

**Variation of Deformation with different parameters**

Figure 4 shows the variation of deformation $D$ with $E$, $r_o$, $\gamma$ and $\varepsilon_m$. The deformation from simulations was calculated using its definition (Eq. (20)). $L$ and $B$ (Fig. 3) were calculated by finding the coordinates of points on the vertical and horizontal axis where the color function $C$ becomes zero. The variation is nearly linear with $E^2$, $r_0$, $1/\gamma$ and $\varepsilon_m$ as suggested by Eq. (20). When $D << 1$, the deformation from our simulations closely mimics the theoretical predictions. However at higher $D$, LBM predicts a larger deformation compared to theory since Eq. (20) was derived under the assumption of small deformation and hence is only valid for small deformations. This deviation has also been observed in earlier studies [10, 17, 22]. The difference in theoretical and LBM predicted deformation at small radii, however, is due to error in finding the exact value of $L$ and $B$. Since the coordinates of the point where color function $C$ exactly becomes zero are determined by linear interpolation between adjacent grid values, the percentage error in calculating $L$ and $B$ is larger when the radius is small.
FIGURE 4: VARIATION OF DROPLET DEFORMATION $D$ WITH (a) ELECTRIC FIELD $|E|$, (b) DROPLET RADIUS $r_o$, (c) INTERFACIAL TENSION $\gamma$ and (d) INNER FLUID PERMITTIVITY $\varepsilon_{in}$ (ALL PROPERTIES IN LB UNITS) - THEORETICAL [18] & USING LBM SIMULATIONS. ($R = S = 2, r_o = 25, |E| = 0.235, \varepsilon_{in} = 0.02, \gamma = 0.01$ UNLESS THE PARAMETER IS VARIED)

Induced Velocity Field

Since tangential stresses cannot be supported by the fluid interface, the tangential electric stresses at the drop interface set up a velocity field in order to balance them with viscous stresses. The theoretical flow field equations lead to the following solution:

$$u_{r,in} = (r^3 - r) \cos 2\theta$$
$$u_{\theta,in} = (r - 2r^3) \sin 2\theta$$
$$u_{r,out} = (1/r - 1/r^3) \cos 2\theta$$
$$u_{\theta,out} = -(1/r^3) \sin 2\theta$$

(22)

Here the radial distance $r$ is expressed in units of $r_o$, and velocities are in units of characteristic velocity $u^*$: $u^* = \frac{R - S}{2S(1 + R)^2} \frac{\varepsilon_{in} E^2 r_o}{\mu_{in} + \mu_{out}}$ (23)

The nature of the velocity field depends on the sign of $R$-$S$ (Eq. (23)). If $R$>$S$, the flow enters from a direction perpendicular to the electric field and is expelled along the equatorial axis. If $R$<$S$, the flow occurs in the reverse direction. The radial and azimuthal components of the velocity along the equator are shown in Fig. 5(a). A distinct feature of the velocity field is that the azimuthal component of velocity at equatorial axis is identically zero. Clearly the velocities obtained by LBM simulation and the theoretical predictions are in good agreement with each other inside the drop ($r < r_o$) under the low deformation limit. Outside the drop, the LBM predicted
velocities deviate from the theoretical values since the theoretical analysis assumes an infinite domain with no boundaries for the outer fluid whereas in LBM simulation, the outer fluid is bounded \((r_{\text{max}} \approx 3r_0)\) in LBM simulation as shown in Fig. 5). The velocities in LBM simulation vanish to zero at the boundaries but the theoretical velocities do not.

From the theoretical flow field equations (Eq. (22)), it is clear that at the interface \((r \approx r_e)\), the radial velocity vanishes. The flow velocities at the interface were computed in LBM simulation by noting that at the interface the color function \(C=0\). These velocities are compared with the theoretical values in Fig. 5(b). The LBM predictions are fairly close to the theoretical values and the LBM predicted radial velocity is very close to zero.

**Flow in T-junction microfluidic device**

The developed model was used to simulate droplet formation in a T-junction in the presence of an electric field. The two fluids used were silicone oil and water. Electrodes positioned at specific locations, as shown in Fig. 6, in the T-junction set up the electric field required. The boundary conditions used were constant potential at the electrodes and vanishing normal component of electric field at the walls of T-junction (i.e. \(E \cdot n = 0\)). A constant pressure was maintained at the exit, with fully developed velocity profiles at the inlets.

![Electrode edge](image1)

**FIGURE 6: SIDE VIEW OF A T-JUNCTION**

To convert physical quantities such as T-junction width \((50 \mu m)\), interfacial tension \((0.045 N/m)\) and density \((1000 kg/m^3)\) to LB units, first a set of reference quantities were chosen to non-dimensionalize them. The width of main channel was taken as reference length, the density of water as reference density and outlet pressure as reference pressure. These non-dimensional quantities were then converted to LB units by discretizing the reference length and the reference time \([21]\) such that the maximum Mach number<0.3. Simulations were carried out for \(Ca=0.01\), \(Re=0.225\) at three different flow rate ratios \(Q=1/5, 1/10\) and \(1/20\). For each case, droplet size and frequency of generation were recorded both with and without the electric field. The droplet size is simply the distance between the two ends of the droplet when it is in the main channel. The frequency of generation was measured by observing the change in color function \(C\) at a point near the exit of the T-junction over time.

Figure 7 and 8 show the variation of droplet size and formation frequency with applied electric field at different flow rate ratios \(Q\).
On applying an electric field, generally a reduction in droplet size and increase in formation frequency was observed. Reduction in the size of droplets and increase in frequency of formation is due to an early pinch-off of the dispersed fluid in the presence of electric field. As the dispersed fluid approaches the point of confluence with the continuous phase in the main channel, the applied electric field causes polarization at the interface leading to coulombic and dielectrophoretic forces on the interface. Since water (dispersed phase) is attracted to the high electric field region [15], it moves towards the edge of the upper electrode (Fig. 6) where electric field is maximum. As a result, the neck of the dispersed fluid gets thinned, assisting in an early pinch off (Fig. 10(b)). Figures 10(a) and (b) show the difference in the mechanism of droplet formation in a T-junction channel in the absence and presence of electric field. Without an electric field, the droplet formation is due to the effect of pressure forces exerted by the continuous phase on the dispersed phase (Fig. 10(a)). In the presence of electric field, electric forces also help in the breaking up of the fluid thereby forming droplets.

From Fig. 7 (resp. 8), it can be seen that there is a local minima (maxima) in the plot at an intermediate value of electric field (|E|=0.1). This is explained as follows. With increase in electric field above a threshold value, the dispersed phase starts getting pinned to the electrodes as it enters the main channel (before breakup). On comparing figures 9(i) and (iii), it can be seen that the pinning at the upper electrode results in accumulation of more volume of dispersed phase in the main channel before droplet formation. The same pinning effect causes a decrease in frequency of droplet formation near the threshold electric field. However, this deviation in behavior is only noticed while transitioning from low electric field (no pinning) to high electric field (when pinning begins).
CONCLUSIONS

A lattice Boltzmann fluid dynamics framework has been developed which incorporates the effects of both electrohydrodynamic and interfacial forces. This model has been validated by comparing the results obtained for benchmarking problems like static droplet test and a leaky dielectric drop in an electric field. This was then successfully employed to the problem of interest.

Results show that it is possible to increase droplet formation frequency and reduce its size in a T-junction by applying an electric field. This arms us with tools to achieve better control over the droplet parameters without changing the flow rate ratio, capillary number and geometry of the T-junction.
ACKNOWLEDGMENT

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REFERENCES


