Proceedings of IMECE2005
2005 ASME International Mechanical Engineering Congress and Exposition
November 5-11, 2005, Orlando, Florida USA

IMECE2005-81757

FLOW INDUCED DYNAMICS OF A PINNED DROPLET ON THE SURFACE OF CHANNEL

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ABSTRACT

Dynamic behavior of a droplet adhering to the surface of a channel has been modeled under the influence of surrounding fluid. The numerical solution is based on solving Navier-Stokes equations for Newtonian liquids. The study includes the effect of interfacial forces with constant surface tension, also effect of adhesion between the wall and droplet accounted by implementing contact angle at the wall. The Volume-Of-Fluid method is used to numerically determine the deformation of free surface. Droplet deformation and final shapes have been predicted. A reduction in the surface tension allows the droplet to deform much easier. However, an increase in the fluid viscosity, although increases the shear force on the droplet, may not result in the deformation at high surface tension. It is shown that deformation of droplet significantly influences structure of channel flow. Effects of liquid droplet and channel fluid properties, namely density and viscosity, inlet velocity, surface tension and channel geometry on dynamics of the problem have been studied. Two different outcomes have been considered: the first one droplet with equilibrium shape and the other one when breakup of the droplet occurs. The border line between the disintegration region and equilibrium region is determined for different droplet surface tensions.

Keywords: Free surface flow; Volume-Of-Fluid; Droplet dynamics in channel flow; Droplet displacement; Droplet breakup;

INTRODUCTION

Multiphase flow involving droplets sitting on a surface of a channel is a common situation encountered in many engineering and scientific problems, including distillation processes, liquid water droplets in the channels of PEM fuel cells etc. Depending on the nature of application, the droplet needs to be kept on the surface or removed. In either case, it would be of value to know the effects of various parameters influencing the critical condition for the droplet.

The specific problem of a droplet on a surface surrounded by an immiscible fluid undergoing a motion has attracted the interest of many researchers and has been the subject of many fundamental fluid mechanics studies. In a series of studies by Dussan V. [1, 2] the effects of external shear flow over an attached droplet has been considered. She determined the yield condition for the critical capillary number as a function of contact angle hysteresis (the difference between the advancing and receding contact angles). The study is based on asymptotic theory valid for very small contact angle hysteresis limited to weak shear flow using lubrication approximation. In the approach by Durbin [3] the wind force needed to displace an adhering droplet from solid surface is sought by considering a 2-dimensional model. By considering the inertia of the surrounding fluid the critical force is given based on the Weber number as a function of contact angle hysteresis. However this study has considered the cases when surrounding fluid is inviscid and droplet is at rest. Feng and Basaran [4] studied a 2-dimensional bubble attached to a slot under shear flow by combining finite element analysis and an iterative method for velocity field and the shape of free surface. They have concluded that the structure of the flow field depends on the Weber number $We = Re\, Ca$. They observed separation of the flow behind the droplet and also an increase in the length of the eddy by increasing Reynolds number. Their study has restricted to low capillary numbers and had no yield conditions based on the capillary numbers. Li and Pozrikidis [5] have studied shear flow over an attached three-dimensional droplet using a boundary-integral method. They have determined the droplet profile by following the dynamic behavior of the interface until a steady shape reached. Effects of capillary number, droplet volume and the shape of contact line have been examined. More deformation for the droplet attached to the wall has been observed compare to the identical freely suspended droplet. Lower critical capillary number for continuous deformation of droplet reported for larger droplet with elliptical contact line. Only droplets and fluids with identical densities have been considered and data is presented for a very limited range of parameter values. In addition only the case of Stokes fluid has been studied.

In the study of Dimitrakopoulos and Higdon [6] the yield condition for a droplet adhering to a plane under shear flow considering the influence of contact angle hysteresis has been determined, including the effects of gravity. It was shown that as gravitational forces increase, the critical *Ca* for continuous deformation of the droplet decreases. Unlike the conclusion by Dussan [2] stating the critical capillary number is independent of the droplet viscosity, they have demonstrated that the behaviors of viscous and inviscid droplet are qualitatively different. Increasing the advancing contact angle for viscous droplet leads to an increase in the critical capillary number, while for inviscid droplets it leads to decrease in the critical capillary number. Scheleizer and Bonneacaze [7] considered the dynamics behavior and stability of a two-dimensional drop between parallel plates in the absence of inertial and gravitational forces. In their studies, they allowed the no-slip boundary condition to be relaxed in order to examine the effects of allowing the droplet to slip. They have presented the shape deformation of the interface for a range of capillary numbers, droplet to surrounding fluid viscosity ratios, and droplet sizes. The deformation of the interface has increased with increasing the capillary number, viscosity ratio, and droplet size up to a certain critical value, after this critical value there is no steady shape exists. In a more recent study, Dimitrakopoulos and Higdon [8] expanded their previous works by considering the displacement for three-dimensional fluid droplets in a pressure –driven flow. Their study attempted to obtain the optimal shape of the contact line which yields the maximum flow rate for which a droplet adheres to the surface. They have observed that when the viscosity of the droplet increases, lower flow rates are needed to displace the droplet from the surface. Limitations of the applied methodology have restricted most of these investigations to the creeping flow limit. For example limitations of the commonly used boundary integral methods have restricted the problem to follow the boundary between two fluids. Nothing is known about the surrounding fluid, flow circulation inside the droplet and their effects on the dynamics of the droplet. The deformation of droplets and their response to shear flow considering the effects of inertia has been an open problem in fluid mechanics. The study done by Fung and Basaran [4] is the only available reference in literature considering the bubble on the surface in finite Reynolds numbers. However, they have limited their study to the case of a bubble with zero viscosity on the surface in a small range of capillary number. The common problem of viscous droplets on a surface has never been addressed.

Our goal is to provide a comprehensive solution for the problem of a droplet adhered on a surface to analyze and develop insight into the dynamics of droplet deformation and the response of the droplet under shear flow at finite Reynolds numbers. Our novel numerical approach enables us to consider the properties of the droplet and the surrounding fluid which correspond to their properties in reality. As an example we are able to address the condition have never been approached like water liquid droplet on the surface with air as the surrounding fluid.

In this paper, we consider a 2-dimensional droplet pinned to the solid surfaces of a channel. The physical consequence of a pinned droplet is that the droplet intersects the solid surface at an arbitrary contact angle without causing the migration of the contact line. This can be true in reality only when the value of the contact line lies in a certain range. This may be achieved in practice by choosing solid materials of appropriate wettabilities.

NOMENCLATURE

L	Channel length, m
H	Channel height, m
R	Droplet radius, m
U	Maximum inlet velocity, m/sec
F	Volume fraction
P	Non-dimensional Pressure
L_c	Droplet characteristic length
D_{max}	Droplet surface maximum distance from the center
Re	Reynolds number
Ca	Capillary number
μ	viscosity, kg/m.sec
ρ	density, kg/m^3
α	viscosity ratio(droplet liquid over channel fluid)
λ	density ratio(droplet liquid over channel fluid)
σ	surface tension, N/m

NUMERICAL METHODOLOGY

We consider an incompressible Newtonian fluid flow in a channel with a constant viscosity of μ and density of ρ that is flowing past a droplet with viscosity αμ, and density λρ sitting on the bottom surface of the channel, as shown in Fig. 2. The interface that separates the droplet and the flowing liquid has a constant surface tension σ. The droplet initially has a semicircular shape with radius ***R***. The radius and the width of the channel are made dimensionless by the length of the channel, L. The boundary conditions are set as follows. The top and the bottom boundaries are no-slip boundaries. The inlet boundary has a parabolic velocity profile with a maximum velocity of ***U***. For the outlet boundary, an outflow (no-gradient) boundary condition is applied.

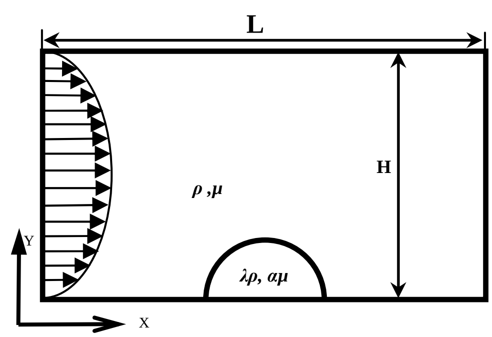


Fig.1: Schematic diagram of attached droplet in the channel.

We have used unsteady incompressible Navier-Stokes equations in two dimensions with fluid interfaces to simulate the motion of an attached droplet under a shear force. A volume-of-fluid (VOF) method, along with a Piecewise Linear Interface Calculation (PLIC) is used to capture the interface motion. It is assumed that the fluids are immiscible without phase change. The velocity field is continuous across the interface, but there is a pressure jump at the interface due to the presence of the surface tension. Following the VOF method by Hirt and Nichols [9], the advective equation for the volume fraction, F, is used to calculate the droplet deformation. The governing equations are (neglecting the gravity):

$$\frac{\partial u_i}{\partial x_i} = 0 , \qquad (1)$$

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0 , \qquad (2)$$

and

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} - F^{st}.\hat{i} + \mu \frac{\partial^2 u_i}{\partial x_j^{\,2}} . \qquad (3)$$

u_i's are the velocity components, and t and x_i are time and space coordinates, respectively. F is the volume fraction of the fluid. It is zero where only fluid 2 exists and it is one where only fluid 1 exits. p is the pressure, $\hat{i}$ is the unit vector in the i^{th} direction, and ρ and μ are the mixture density and viscosity defined as:

$$\rho = \rho_2 + F(\rho_1 - \rho_2) \qquad (4)$$

$$\mu = \mu_2 + F(\mu_1 - \mu_2) \qquad (5)$$

where, ρ_1 and ρ_2, and μ_1 and μ_2 are densities and viscosities of fluids 1 and 2, respectively.

For the surface tension forces, we use the Continuum Surface Stress (CSS) model [10] which is defined as:

$$F^{st} = \sigma \nabla \cdot (|\nabla F| \mathbf{I} - \frac{\nabla F \otimes \nabla F}{|\nabla F|}) \qquad (6)$$

where **I** is identity matrix. The CSS model reformulates surface tension into a volumetric force. To apply this formulation, one needs to spread the surface tension force over the fluid in the vicinity of the interface. The interface normal vector is proportional to the gradient of the volume fraction F. A better estimation of this normal vector can be obtained by evaluating the gradient using a smoothed volume fraction, $\tilde{F}$, equivalent to employing a spatially weighted gradient operator. We have used a formulation similar to Bussman *et al.* [11] for the smoothing kernel. If a pressure based numerical method is used (as it is the case in this paper), then the Poisson equation should be solved. The Poisson equation is obtained by taking the divergence of the momentum equation, Eq. (3), and using the continuity equation, Eq. (1), to simplify it.

A modified version of SURFER code [10, 12, 13] is used in this work. The details of the numerical method based on VOF-PLIC and Chorin's projection method for a semi-implicit Navier-Stokes solver are given in [9] and are not repeated here. The adhesion between the wall and the droplet has been accounted by implementing a contact angle at the wall. Wall adhesion is a surface force acting on the fluid interface at points of contact with the wall. This force is calculated for the cells within the proximity of the wall, except that a boundary condition is applied to the free surface unit normal prior to evaluating the force. Details of the implementation of the method are given by Kothe *et al.* [14]. Equations are solved in a uniform grid in both x and y directions. A grid dependency study showed that acceptable resolution is obtained by using 25 cells per radius.

RESULTS AND DISCUSSION

When a fluid is forced to pass a stationary droplet, shear forces start to deform the droplet. Inertia and shear forces resulting from the surrounding fluid as well as pressure difference across the droplet try to deform and move the droplet in the direction of the flow. The surface tension forces tend to keep the droplet spherical and attached to the surface. The geometry of the system also plays an important role in the droplet deformation. A droplet in the channel acts as a barrier against the flow. Therefore, the pressure difference across the droplet increases as the relative height of the droplet to the channel width increases. This pressure difference tends to move the droplet in the direction of the incoming flow. A typical pressure contour has been shown in Fig.2. Incoming channel fluid moves across the droplet, causing a significant pressure difference buildup across the droplet due to the droplet blockage (a low pressure region at the upstream and a high pressure at the downstream). The contour levels shown to the right of the Fig.1 represent non-dimensional pressure.

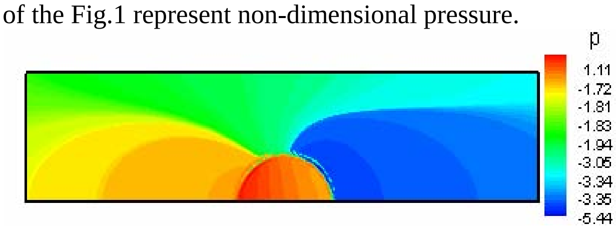
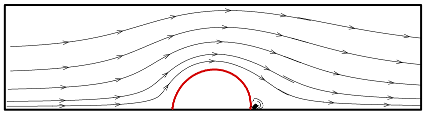


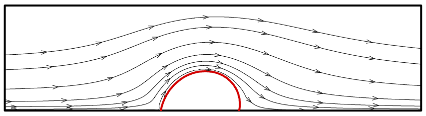
Fig. 2: Pressure contours across a droplet in a channel flow.

For the simulation, a liquid droplet with density of $\lambda\rho$ and viscosity $\alpha\mu$ is used. Density and viscosity of the channel flow are scaled based on the properties of liquid water with coefficients λ, and α, representing the density ratio, and the viscosity ratio, respectively. Initially, droplet radius is a quarter of the channel width, which itself is 1/8 of the channel length. Contact angle between the droplet and the wall is 90 degrees. A parabolic velocity profile with a maximum inlet velocity of U_{max} is implemented for the incoming gas. This velocity ranges between 1.5 *m/sec* to 5 *m/sec*. Three values for the surface tension coefficient have been used during the simulations, 0.073 *N/m*, 0.063 *N/m*, and 0.0073 *N/m*.

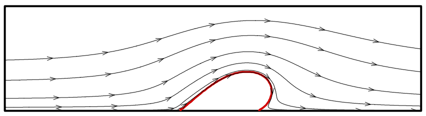
Discussed in detail in Golpaygan and Ashgriz [15], surface tension considerably influences the final shape of the droplet on the surface of a channel. In Fig. 3, the effects of surface tension on a droplet equilibrium shape have been compared. The deformation of the droplet increases by decreasing surface tension. The channel flow has the maximum inlet velocity of 1.5 m/sec with λ=1000, and α =1. Streamlines in Fig. 3 show that for droplets with small surface tension coefficients, streamlines conform to the droplet deformed shape. However, at relatively large surface tensions (Fig. 3-a, σ= 0.073*N/m*) a small eddy is formed downstream of the droplet. High surface tension forces do not allow the droplet to deform. Therefore, the droplet acts as a solid barrier against the incoming fluid and the available space for the surrounding fluid remains unchanged. We have used a Capillary number, ***Ca*** = $\mu U/\sigma$, defined based on the channel fluid viscosity, and a Reynolds number, ***Re*** = $\rho UD/\alpha\mu$, defined based on channel fluid density but droplet viscosity, to describe the effect of fluid properties and the channel geometry on the droplet deformation. The Capillary number represents the ratio of shear forces to surface tension forces. On the other hand, the Reynolds number represents the ratio of inertia forces to viscous forces.



(**a**) σ =0.073N/m



(**b**) σ =0.0365N/m



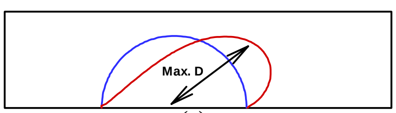
(**c**) σ =0.0073N/m

Fig. 3: Channel flow structure passing a pinned droplet with Re=46.

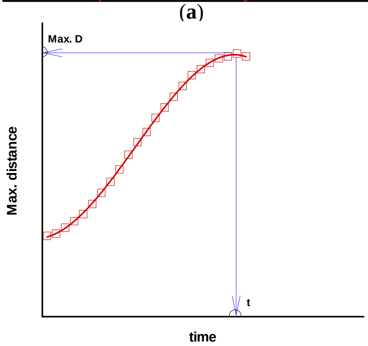
A characteristic length for the droplet is defined as follow to keep track of droplet deformation. Figure 4-shows the initial and the final equilibrium shapes of a droplet in a channel flow. In addition, Fig. 4-b shows the time evolution of the maximum distance between the droplet surface and the center of the droplet. The largest value of this maximum distance, $\boldsymbol{D_{max}}$, is used as a scale for the droplet deformation and its value is used for comparison in our case study. The characteristic length for the droplet deformation is defined as

$$L_c = \boldsymbol{D_{max}}/\mathbf{R}$$

where **R** is the initial droplet radius.



(a)



(b)

Fig. 4: (a) Initial and equilibrium shapes of a droplet with Max distance from the center, (b) changes of Max distance of droplet surface with time.

Increasing the Capillary number by decreasing the surface tension increases the characteristic length of the droplet until no equilibrium shape can be achieved. Decreasing surface tension from 0.073 to 0.0365 and then 0.0073 N/m has increased droplet characteristic length from 1.08 to 1.12, and then 1.55 (Fig. 3).

If the flow is strong enough, the distorting stresses outweigh the forces due to the presence of surface tension and adhesion between the droplet and the wall. Therefore, a steady state condition, which requires a balance of forces on the interface, can no longer be achieved. Disintegration of the free surface is the usual consequence of this imbalance. In this situation a droplet may breakup into several fragments as shown in Fig. 5.

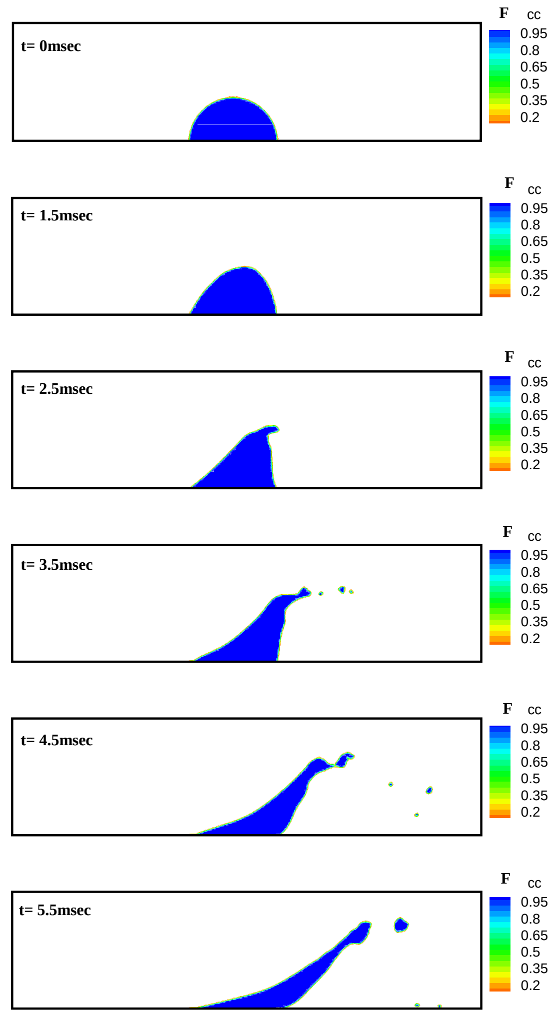


Fig.5: Deformation and disintegration of an attached droplet.

The results shown in Figs. 5 correspond to a droplet pinned to the surface of the channel with a density of 1000 kg/m^3 and viscosity of 0.001 *kg/ms*. The channel flow has maximum inlet velocity of 5 *m/sec* with $\lambda=20$, and α =1. The coefficient of surface tension is 0.073*N/m*. The corresponding Capillary and Reynolds numbers are 0.07, 7812.5, respectively.

When the flow is not strong enough, a steady state condition based on the balance of forces resulting from inertia and shear stresses one side and surface tension and pressure difference across the droplet in the other side will be reached. In Fig. 6 structure of the flow in the channel and deformation of the pinned droplet until the point it reaches an equilibrium shape has been compared. As the incoming flow starts developing, it encounters the droplet. A pressure difference across the droplet builds up as shown in Fig. 6. The droplet starts to deform and its characteristic length increases to 1.367 and then 1.55 at t=10msec and t=17msec. The forces are in equilibrium after this point, therefore no changes in the characteristic length can be observed (at t=17msec, L_c=1.55, and at t=20msec, L_c=1.55).

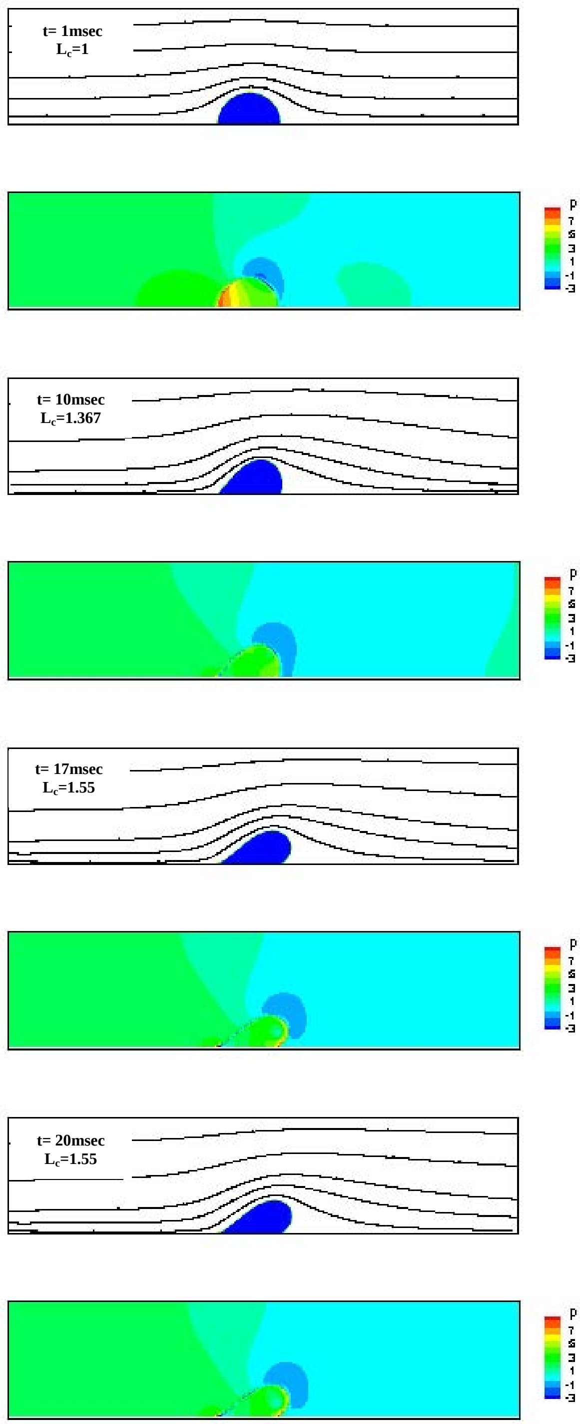


Fig. 6: The flow structure and pressure contours for a droplet reaching an equilibrium shape.

In the results shown in Fig. 6 the droplet liquid has a density of 1000 kg/m^3 and viscosity of 0.001 *kg/ms*. The channel flow has a maximum inlet velocity of 1.5 *m/sec* with $\lambda=200$, and α =1. The coefficient of surface tension is 0.01*N/m*. These corresponding Capillary and Reynolds numbers are *Ca*=0.15 and *Re*=234.37.

Droplet deformation and the channel flow structure with different viscosities are compared in Fig. 7, for a constant surface tension coefficient of σ=0.0073*N/m*. Recall that α in this figure represents the ratio of the viscosity of the droplet to that of the channel fluid. The characteristic length of the droplet increases with increasing the Capillary number. In Fig. 8-a, the channel fluid has a higher viscosity compared to the other cases; therefore, the droplet deforms more. Deformation of the droplet prevents flow separation in the channel. Flow separation and recirculation eddies are observed when the viscosity of the channel fluid is decreased.
The size of the separated eddy increases with decreasing the viscosity of the channel fluid. At small Capillary numbers, the streamlines retain their shape around the droplet while the droplet is deforming. The shape of the separated eddies are similar to the ones that occur in a flow passing around a circular obstacle. However, Fig. 7 indicates that the appearance of the flow separation and the size of the separated eddy are not solely determined by the *Re* number. For example, in Fig. 7-c, a much larger eddy compared to the other cases is observed, when *Re* =46 in all three cases. Therefore droplet deformation is an important factor in the generation of eddies.

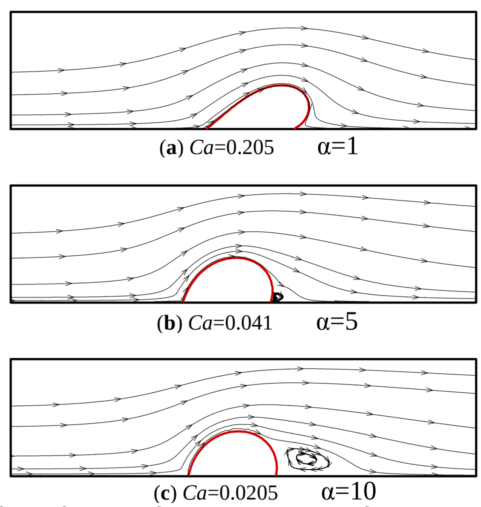


Fig. 7: Effects of channel fluid viscosity on the flow structure.

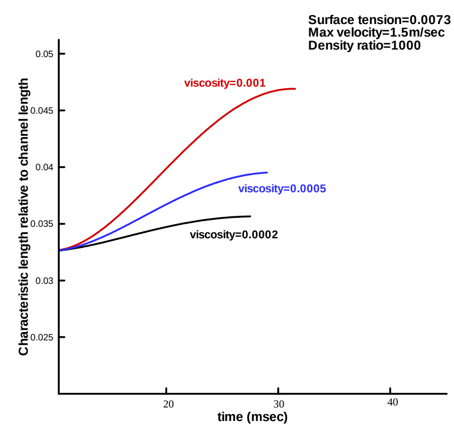


Fig. 8: Effects of channel fluid viscosity on the characteristic length of the droplet.

The results indicate that the viscosity is an important parameter in the droplet deformation. Figure 8 shows the time evolution of the droplet characteristic length for viscosities of 0.001, 0.005 and 0.0002 *kg/m.s*. As expected, decreasing the absolute viscosity decreases the characteristic length. In addition, the time to reach the maximum droplet deformation decreases when the viscosity is changed from 0.001 to 0.0002 *kg/m.s*. In more viscous fluids, the droplet deforms to conform to the flow resulting in less flow separation.

The characteristic length has been used to distinguish between the two cases where the droplet reaches an equilibrium shape or the one when no-equilibrium shape exists. As shown, in the equilibrium shape, the characteristic length of droplet increases until the steady state shape of droplet obtained. In the non-equilibrium case, the droplet continues to deform until disintegration occurs.

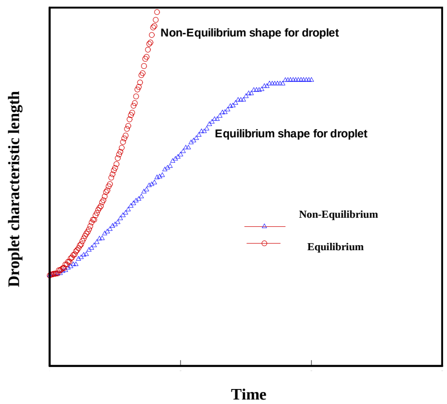


Fig. 9: Changes in droplet characteristic length versus time for droplet with equilibrium and Non-equilibrium shape.

As noted earlier, pinned droplets under the influence of a channel flow may either breakup or reach an equilibrium shape, depending on the properties of droplet and channel flow. The border line between these two regions is shown in Fig. 9. A liquid water droplet with density of 1000 kg/m^3 and viscosity of 0.001 *kg/ms* is considered on the surface of a channel. The coefficient of surface tension is equal to 0.0365*N/m.* For a specified R/H (droplet radius over channel width), the Reynolds number increases until the droplet disintegrate into small fragments. The inertia of the channel flow increases by decreasing the density ratio, λ.

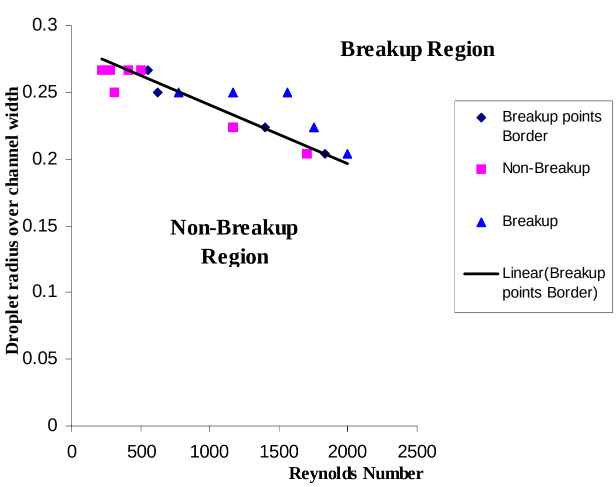


Fig. 9: Breakup border line for *Ca*=0.137.

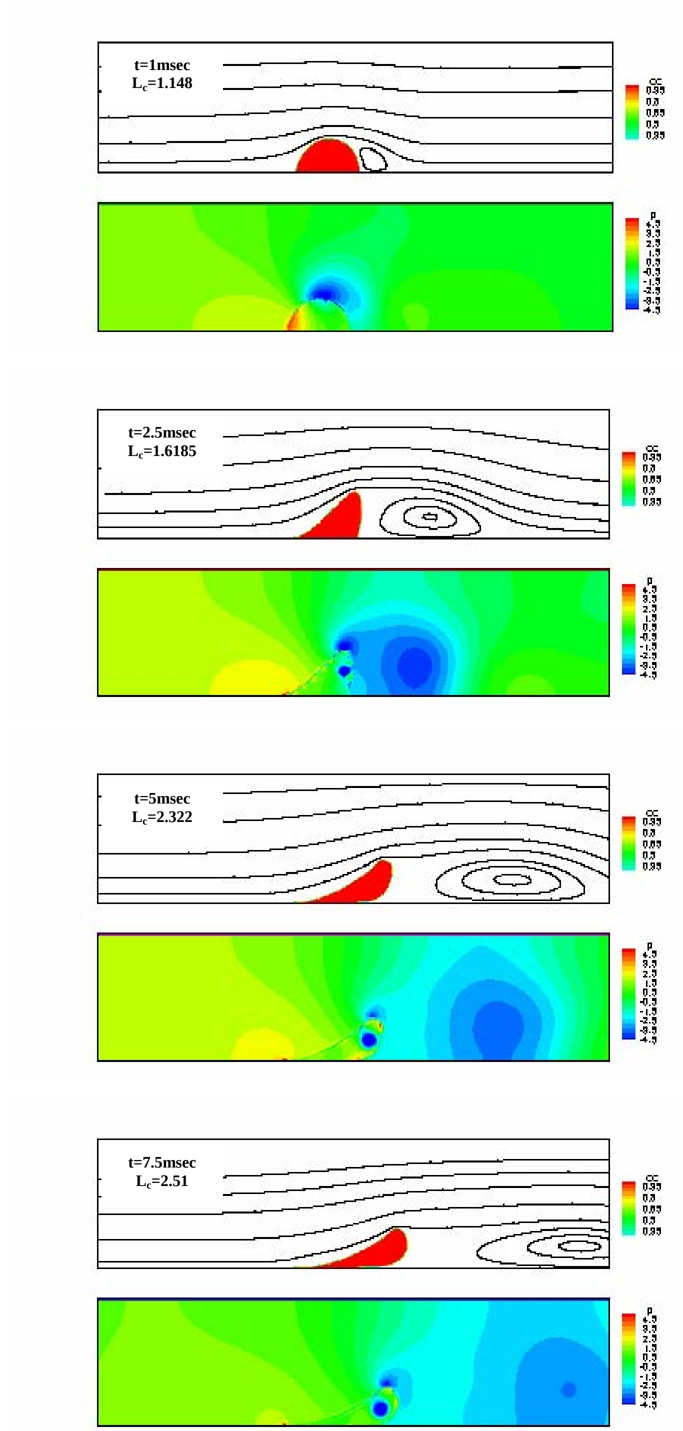


Fig. 10: The flow structure and pressure contours for a droplet detaching from the surface.

Droplet and channel flow properties, channel geometry and the rate of incoming channel flow also affect the mechanism of droplet breakup. Differing from the disintegration effects shown in Fig. 5, Fig. 10 shows the channel flow deforming the droplet continuously until the detachment of the droplet from the surface occurs. The high surface tension of the droplet (σ=0.073N/m) in the case corresponding to Fig. 5, prevent droplet from initial deformation. However the interfacial tension forces can no longer balance the viscous and inertial forces, so the deformations become unstable and the droplet breakup. Compare to disintegration of the droplet (Fig. 5), the density ratio has been increased to λ=80 in Fig. 10. This change decreases inertia of the channel flow. The droplet deforms to conform to surrounding fluid; however balance of forces still does not exist. The breakup involves detachment of the droplet from the surface. As shown in Fig. 11, increasing droplet radius decreases the Reynolds number at which breakup of the droplet occurs. This breakup point moves to higher Reynolds number when the surface tension decreases. As an example, at droplet radius over channel width of 0.25 droplet breakup occurs at Reynolds number of 625 when the surface tension coefficient is 0.073 N/m. The breakup of the droplet occurs at *Re*=1562 when the surface tension coefficient decreases to 0.0365 N/m.

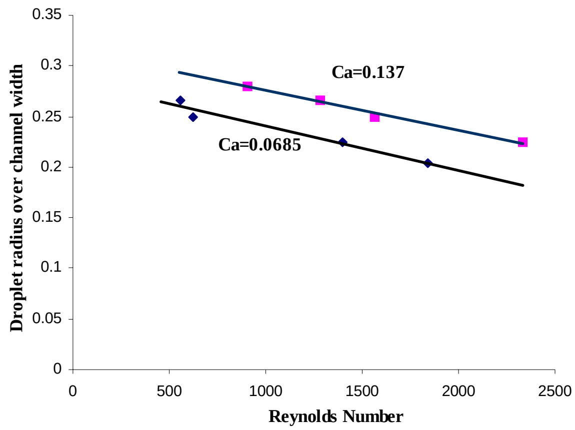


Fig. 11: Effects of the Capillary number on the breakup border line

SUMMARY AND CONCLUSION

A two-fluid numerical model has been employed to study dynamics of a pinned droplet on the surface of channel. To keep track of interface deformations and droplet motion Volume-Of-Fluid method has been used. Surface tension is modeled as a volume force acting in the vicinity of the free surfaces. Our novel numerical approach enables us to study cases which have never been approached before, including pinned droplet on the surface when λ=1000(density ratio of droplet over the channel fluid) with surface tension as high as 0.073N/m. The surface tension effects, as well as the channel fluid velocity and viscosity are represented through the Capillary number ($Ca = \mu U/\sigma$). Reynolds number is used as another parameter to indicate the importance of the inertia of flow in the channel and the fluid viscous effects.

The inertia and shear forces resulting from the moving outer flow try to overcome the forces resulting from surface tension and the adhesion of the droplet to the surface. Liquid droplet and channel fluid properties, namely density and viscosity, inlet velocity, surface tension and channel geometry determine whether the droplet just deform and remain stationary or disintegrate from the surface. A comprehensive study is conducted, covering a wide range of viscosity ratios, density ratios, surface tension and droplet sizes. It is shown that deformation of the droplet significantly influences the structure of the flow in the channel. At a constant Reynolds number, the size of separated eddies increase with increasing surface tension.

The characteristic length of the droplet is used to compare droplet deformation due to changes in the surface tension, viscosity and density ratios. Based on these properties the droplet either reaches an equilibrium shape or breakup. Two different breakup mechanisms have been distinguished: unstable deformation follow by breaking of droplet into small fragments, and the other continuous deformation and detachment from the surface. At a specified Capillary number, the border line between breakup and no-breakup regions linearly relates to the Reynolds number and the height of the droplet in the channel. This breakup border line moves toward higher Reynolds number when the surface tension decreases

ACKNOWLEDGMENTS

The authors acknowledge support provided by Canada's Auto 21 Network for Centers of Excellence.

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