ABSTRACT
In this paper we present a first order study of liquid water detachment and entrainment into air flows in hydrophobic microchannels. A silicon based microfabricated test structure was used for this purpose. It consists of a 500 µm wide by 45 µm deep U-shaped channel 23 mm in length through which air is flown. The structures are treated with a Molecular Vapor Deposition (MVD) process that renders them hydrophobic with a nominal contact angle of 108° (in situ contact angles inside the channels are measured directly during testing). Liquid water is injected through a single side slot located two-thirds of the way downstream from the air channel inlet. The side slot extends the whole depth of the air channel while its width is varied from sample to sample. Visualization of the water slugs that form as water is injected into the air channel was performed. Slug dimensions at detachment are correlated against superficial gas velocity.

Proper dimensionless parameters are postulated and examined to compare hydrodynamics forces against surface tension. It is found that for \( Re \) below 200 slug detachment is dominated by pressure gradient drag arising from confinement of a viscous flow in the channel. On the other hand, for \( Re \) above 200 the predominant drag is inertial in nature with stagnation of the air due to flow obstruction by the slugs.

KEYWORDS
Microchannels, two-phase flow, droplet detachment, slug detachment, fuel cells.

NOMENCLATURE
- \( A_{\text{drop}} \) slug cross-sectional area [m²]
- \( C_D \) slug form drag coefficient
- \( D \) characteristic dimension [m]
- \( D_h \) effective hydraulic diameter [m]
- \( f \) friction factor
- \( g \) gravitational acceleration [m/s²]
- \( h \) slug cross width [m]
- \( H \) channel in plane dimension [m]
- \( l \) slug length [m]
- \( U_{\text{air}} \) air superficial velocity [m/s]
- \( V \) characteristic velocity [m/s]
- \( W \) channel out of plane dimension [m]
- \( \mu \) dynamic viscosity [Pa·s]
- \( \mu_{\text{air}} \) air dynamic viscosity [Pa·s]
- \( \rho \) density [kg/m³]
- \( \rho_{\text{air}} \) air density [kg/m³]
- \( \rho_w \) water density
- \( \sigma \) water surface tension [N/m]
- \( \theta_a \) advancing contact angle
- \( \theta_r \) receding contact angle

INTRODUCTION
Water management is one of the key aspects related to Proton Exchange Membrane Fuel Cell (PEMFC) operation. With the push for miniaturization of PEMs to complement portable devices and the use of microchannels to improve their performance [1], issues related to water transport become increasingly more important. Understanding how water makes its way into and out of the microchannels can lead to the development of successful strategies and designs that minimize flooding but allow proper hydration of the electrolytic membrane. An important aspect in this process is the detachment and entrainment of liquid droplets into confined air streams from hydrophobic surfaces.

The electrodes in a PEMFC consist of a porous material known as the Gas Diffusion Layer (GDL), a hydrophobic medium that allows diffusion of the reactive gases to the catalytic sites while rejecting liquid water. Liquid water formed in the cathode site that percolates through the GDL collects in the form of droplets in its surface. In a best case scenario the droplets are removed by the incoming stream of air and exhausted through the channel outlet. However, in some instances the water droplets grow unimpeded until they fill the channel and clog it. It is the goal of this study to determine the air flow conditions that lead to removal of the droplets prior to reaching the critical channel size.
The complexities of water management in PEMFCs have been previously investigated [2-4]. However, most studies have focused on the issue of water flow and transport only in the Membrane Electrode Assembly (MEA) and GDL. Very few studies have been directed towards understanding of the flow behavior in the microchannels, and most are theoretical or computational in nature [5, 6]. Experimental work related to two-phase flow in fuel cell channels is limited and relates mainly to minichannels (mm size) [7] and direct methanol fuel cell systems, with low void fractions [8].

Conversely, the dynamics of phase entrainment in microscale two-phase flows have been addressed for conditions unrelated to fuel cell applications [9-15]. Several studies exist on the departure criteria of bubbles in microchannel boiling flows [10, 11]. There is also a great deal of work on the formation of droplets in two-component liquids flows [10, 11]. More specifically, Mahé et. al [14] and Basu et. al [15] have looked at the sliding and detachment of liquid droplets subjected to shear flows and established a correlation between droplet drag and contact angle hysteresis. However, there is still a need for proper characterization of the parameters that govern droplet detachment in confined geometries. Furthermore, as it will be shown, there seems to be more than one mechanism at play in the detachment of liquid droplets, leading to the formulation of regimes and transition points where different forces are prevalent.

**EXPERIMENTAL STRUCTURE AND SETUP**

A silicon based microfabricated test structure is used to simulate the introduction and formation of water droplets into the microchannels. The structures consist of a 500 µm wide by 45 µm deep U-shaped channel 23 mm in length through which air is flown. Liquid water is injected through a side slot located two-thirds of the way downstream from the air channel inlet. Figure 1 shows the layout of the test structures. The side slot extends the whole depth of the air channel and is therefore 45 µm deep. Two different side slot widths were tested, 10 and 50 µm.

![Figure 1: Test structure layout.](image)

The microfabrication process utilizes a plasma etching process known as Deep Reactive Ion Etching (DRIE) to carve out the air and water injection channels in a silicon wafer substrate. DRIE is also used to create thru holes in the silicon substrate that serve as inlets and outlet for the fluids. A glass cover is anodically bonded to the silicon wafer substrate to allow visualization of the flow and to seal the structure. Figure 2 depicts the microfabrication process flow in detail. Channel depth is roughly controlled by the etching time, but actual depths have to be determined through post fabrication evaluation.

![Figure 2: Microfabrication process: (a) Frontside etching of air and water channels layout. (b) Backside through etch of air and water inlet/outlet ports. (c) Anodic bonding with glass cover.](image)

In order to render the channels hydrophobic, the structures are treated with a Molecular Vapor Deposition (MVD) process developed by Applied Micro Structures, Inc. (AMS). Contact angle measurements carried out on the exterior surfaces of the chip returned values of 108°. In situ contact angles inside the channels are also measured directly during testing.

Testing requires precise metering and control of the air and water flows. Likewise, it must allow for proper visualization of the water slug formation and detachment. Figure 3 shows a schematic of the setup.

![Figure 3: Experimental setup schematic.](image)
chip) are monitored using an Omega mass and volumetric flow meter (model FMA-1600). The pressure drop across the channel is monitored with a differential diaphragm pressure transducer (Validyne DP15TL). The exit is kept open at atmospheric conditions. The system incorporates feedback and can therefore be operated under either pressure or flow rate control. In the tests presented in this paper pressure was treated as the independent variable and air flow rate as the dependent one. Distilled water is supplied and controlled with the use of a Harvard Apparatus Pump 11 single syringe pump. All tests were conducted under constant water flow rate.

For visualization and imaging purposes a Nikon TE2000U inverted epifluorescence microscope was employed. It was operated in reflective white light imaging mode with 4X and 10X objectives. A Roper Scientific 12-bit CoolSNAP ES CCD camera was used for image capture. Figure 4 shows a schematic of the microscope configuration in fluorescence mode.

**Figure 4: Imaging setup configuration.**

**SLUG MORPHOLOGY**

Due to the aspect ratio and geometry of the main microchannel and side slot, the water introduced into the microchannel forms into a pancake like slug or blob rather than a spherical cap (see Figure 5). In an actual PEMFC microchannel it is most likely for water to form into spherical droplets due to the effective GDL pore size and unconstrained geometry of the channels. These differences in geometry and slug morphology affect the actual and relative values of the capillary, inertial and viscous forces involved. However, if they are properly accounted for, the underlying principles behind blob removal are still valid across geometries.

The morphology of the blobs has significant effects on the surface tension, inertial and viscous induced forces particularly through their cross channel and longitudinal extent (see Figure 5). As water is introduced through the side slot, the liquid grows into a pancake shaped slug that remains pinned at the injection site until it reaches a critical size and removal occurs. Quantification of the geometrical parameters of the blobs at this precise instant in time is crucial in the determination of the forces involved during droplet entrainment.

For each flow rate condition these dimensions are measured from the visualization images. Since the slug growth rate and detachment process are too fast for the camera to capture on a single event, we rely on an ensemble average of pictures taken randomly at different stages of the process on different events. Measurements of the cross channel and longitudinal extent of slugs that have separated from the injection slot are taken and averaged over a sequence of 40 images (only images with separated slugs are considered). Tests were conducted in samples with water injection side slot widths of 10 µm and 50 µm. Corresponding water injection flow rates of 50 µL/min and 10 µL/min were used, respectively. The results are plotted in Figure 6 and Figure 7. From these plots it becomes apparent that the cross channel dimension of the blobs decreases linearly with air flow rate/velocity. On the other hand, the longitudinal dimension of the slugs decreases in an inverse power fashion with air flow rate/velocity. It is also apparent that under the conditions tested side slot width and water injection rate have no apparent effects on slug departure criteria. Water injection rate influences the slug entrainment frequency but not its departure size. It is conceivable that under really large water injection rates and velocities other forces, such as inertia of the water, might come into play and affect the criteria controlling the size of the slugs at departure.

**Figure 5: Water slug formation and detachment.** At departure, slugs are characterized by their cross channel (W) and longitudinal (L) extents.

**Figure 6: Slugs cross channel extent as a function of average air inlet velocity.**
FORCE CALCULATIONS AND DIMENSIONLESS PARAMETERS

The dimensions and morphological data collected from the visualization images along with the channel geometry were used to calculate the different forces involved in the microchannel. Representative dimensionless parameters capturing the driving physics behind slug detachment were also evaluated and when appropriate postulated.

Due to the small dimensions of the channels the first parameter to be considered was the Bond number in order to assess the effects of gravity relative to surface tension, which is a predominant force when small dimensions are involved. The Bond number is given by

\[ \text{Bo} = \frac{(\rho_w - \rho_{air}) g D^2}{\sigma} \]  

(1)

where \( D \) is a characteristic dimension representative of the system. The \( \text{Bo} \) number ratio compares gravitational to capillary force. Gravitational forces are important or predominant when \( \text{Bo} \gg 1 \). The largest \( \text{Bo} \) number is obtained by using the largest possible value for the characteristic dimension, \( D \). This can be taken to be the width of the channel or the largest longitudinal slug dimension recorded. In either case \( \text{Bo} \ll 1 \) which means that gravitational effects can be neglected.

Attention is then turn to the other forces involved, particularly the viscous and inertial forces. Traditionally, comparison of the viscous and inertial forces relative to surface tension is done through the Capillary (\( \text{Ca} \)) and Weber (\( \text{We} \)) numbers, respectively. In their standard form they are given by

\[ \text{Ca} = \frac{\mu V}{\sigma} \]  

(2)

\[ \text{We} = \frac{\rho V^2 D}{\sigma} \]  

(3)

The \( \text{Ca} \) number compares the viscous shear stress to the capillary pressure while the \( \text{We} \) number compares inertia based drag to surface tension force. Notice that there is no characteristic lengthscale in the \( \text{Ca} \) number. This is the result of both the shear stress and capillary pressure being based on the same dimension. However, depending on the configuration or geometry of the problem this might not be the case. In such instances a modified \( \text{Ca} \) number must be introduced. The same argument can be made for the \( \text{We} \) number, resulting in modified versions of these numbers that account for specifics of the configuration and geometry of the system. Figure 8 shows a schematic with the channel and slug geometries used for these purposes.

\[ \text{Ca}_{\text{mod}} = \frac{\text{air viscous force}}{\text{surface tension}} \]  

(4)

\[ \text{Ca}_{\text{mod}} \approx \frac{\mu_{\text{air}} U_{\text{air}} (H - h) W l}{2 \sigma (l + h)(\cos \theta_r - \cos \theta_a)} \]  

(5)

\[ \text{Ca}_{\text{mod}} \approx \frac{\mu_{\text{air}} U_{\text{air}} H W l}{2 \sigma (l + h)(\cos \theta_r - \cos \theta_a)(H - h)^2} \]  

(6)

\[ \text{We}_{\text{mod}} = \frac{\text{air inertial force}}{\text{surface tension}} \]  

(7)

\[ \text{We}_{\text{mod}} \approx \frac{1}{2} \frac{\rho_{\text{air}} U_{\text{air}}^2 A_{\text{drop}} C_D}{2 \sigma (l + h)(\cos \theta_r - \cos \theta_a)} \]  

(8)

\[ \text{We}_{\text{mod}} \approx \frac{\rho_{\text{air}} U_{\text{air}}^2 h W}{4 \sigma (l + h)(\cos \theta_r - \cos \theta_a)} \]  

(9)

Figure 9 and Figure 10 show plots of the \( \text{Ca}_{\text{mod}} \) and \( \text{We}_{\text{mod}} \) as functions of inlet air Re number. It is apparent from the \( \text{Ca}_{\text{mod}} \) plot that shear viscous forces are negligible in comparison with surface tension forces and therefore unlikely
to perturb or even deform the slugs. On the other hand for \( Re > 200 \) the \( W_{e mod} \) is on the order of one, suggesting that inertial forces are comparable to surface tension forces and can therefore lead to detachment of the slugs. Nonetheless for \( Re < 200 \) the \( W_{e mod} \) dips below one, such that the inertial force is smaller than the surface tension force in this range. This indicates that a different mechanism must be involved in slug detachment for these flow conditions.

Several things should be noted from equations (6), (12) and (13). First is that, as pointed out before, the effects of constricted geometry by the presence of the slugs are taken into account as an increase in air velocity by the ratio \( w/(w-W) \) and in the calculation of the effective hydraulic diameter, \( D_h \). The product \( fRe \) is also dependent on geometry and as such would be influenced by the change in effective aspect ratio introduced by the slug blockage. However, in this preliminary study we have used a constant \( fRe \) value corresponding to the aspect ratio of the microchannel. Secondly, and perhaps more interesting, is the fact that the \( Dr \) number looks like a \( Camod \) number. However the physics and underlying principles behind the two are quite different.

The \( Ca_{mod} \) compares the viscous shearing force acting on the surface of the slug to the surface tension force. On the other hand the \( Dr \) compares the pressure gradient induced drag force acting on the cross sectional area of the slug to the surface tension force. But this pressure gradient is a result of the viscous shear stresses on the walls of the microchannel and hence its dependence on a shearing-like term in the dimensionless parameter. As such, further examination and comparison between equations (6) and (12) will reveal that in the \( Ca_{mod} \) number only the velocity gradient in the cross width \( y \)-direction and viscous stresses acting on the upper surface of the slug (shearing surface) are relevant. Conversely, in the \( Dr \) number all the velocity gradients and viscous stresses are important, as evidenced in part by the inclusion of the \( fRe \) product.

Figure 11 shows plots of the \( Dr \) as a function of inlet air \( Re \) number. The relevance of the pressure gradient drag decreases with increasing \( Re \) number as evidenced by this plot.
However, at low $Re$ number it is a dominant force and is mostly responsible for the detachment of the water slugs. Figure 12 shows a combined plot of the $Dr$ and $We_{mod}$ numbers against inlet air $Re$ number and regime map for slug detachment. Two regimes and a transition point can be identified in this plot. The transition point occurs at $Re = 200$. For $Re < 200$ slug detachment is dominated by the viscous induced pressure gradient drag while for $Re > 200$ slug detachment is dominated by inertial drag. The first type of drag is generated by the object (slug in this case) being immersed in a pressure gradient field. The second type of drag is generated by the increased pressure at the front of the object (slug in this case) resulting from the deceleration of the air as it encounters an obstruction (slug) in its path.

Figure 11: $Dr$ number as a function of inlet air $Re$ for two different injection side slots widths.

![Dr vs. Re graph](image)

Figure 12: Slug detachment regimes and transition point.

The analysis that has been presented here is of first order and as such is mainly 2D, particularly in terms of surface tension effects. Consideration of contact angle hysteresis has been taken into account in the plane of the image but not so for the out of plane curvature. However, it can be argued by symmetry arguments that the out of plane surface tension effects along the triple contact line tend to cancel each other. As such the out of plane surface tension effects are minimal and can therefore be neglected, especially under a first order analysis. Further studies must be carried out to validate or disprove this argument in a more rigorous analysis, though.

**SUMMARY AND CONCLUSIONS**

We have presented a first order study of the physics behind droplet and blob detachment in microchannels. The channels were microfabricated in silicon and consisted of main channel through which air was flown and a side slot through which water was injected. Water injection created liquid blobs in the main channel that were swept away by the air flow. Experiments were performed to measure the cross channel and longitudinal extents of the slugs at detachment.

Experimental results showed that viscous shearing forces acting on the blobs are negligible compared to surface tension forces. Inertial drag become substantial at $Re > 200$ and in this range is the main force responsible for the detachment of the slugs. At low $Re$ (below 200) a different mechanism is responsible for the entrainment of the slugs into the air flow. Drag created by the pressure gradient across the blob is responsible for detachment of the slugs. The pressure gradient is mainly a result of the viscous shear stresses acting on the wall of the microchannels. The slugs influence this gradient by means of constricting the effective area over which the air must flow.

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