ABSTRACT
The present study is performed to analyze the growth and departure of a water droplet inside a minichannel with air flowing through it. The minichannel is of 1 mm square cross section with a water droplet growing at the top wall and air coming in through the channel inlet. This is a typical situation encountered in the gas flow passages of a PEM fuel cell. The excess water generated in the membrane due to the fuel cell reaction diffuses through the gas diffusion media and enters the gas supply minichannel passages where it gets entrained in the flow. The excess water needs to be removed quickly to prevent flooding of the membrane and gas flow passages which stops the fuel cell operation. The complete Navier-Stokes equations along with continuity equation are solved using the SIMPLE method. The liquid vapor interface is captured using the level set technique. The droplet grows due to flow of water at its base and at the same time is dragged due to the air flowing over it. The droplet growth and its departure are studied for different values water flow rate, incoming air flow rate and contact angle. The droplet departure is found to be hindered by excessive water flow rate and increase in surface wettability.

INTRODUCTION
In the age of global warming and increased environmental concerns fuel cell systems are seen as the future promise for clean and efficient power generation. The basic reaction in a fuel cell involves combination of hydrogen and oxygen to generate electrical energy while water is produced as a byproduct. Proton Exchange Membrane fuel cells (PEMFC) are low temperature fuel cells which uses a solid polymer membrane as the electrolyte are being actively developed for use in cars and buses. It is important to maintain the electrolyte at a correct level of hydration for proper functioning of the fuel cell. The proton conductivity of the electrolyte is directly proportional to the water content whereas too much water can flood the electrodes blocking the pores in the gas diffusion medium (GDM). The excess water generated at the cathode is swept out of the stack by the excess air circulating over the cathode through the channels on the bi-polar plates.

Borreli et al. (2005) obtained high speed images of water droplets moving from two different GDM samples into a simulated PEMFC cathode minichannel. They measured the advancing and receding contact angles and the departure droplet diameters from the side-view images of the departing droplets. The droplets were observed to occur at preferred locations in the GDM and the departure diameter was found to decrease with increasing superficial gas velocity. The receding contact angle was found to decrease with increase in the droplet departure diameter whereas the advancing contact angle remained almost constant.

Trabold (2005) provided an overview of minichannel applications in PEM fuel cells with respect to fuel cell water management. According to him the flow through the channels on the cathode side of the fuel cell where water is produced is complicated since not only two-phase flow is likely to develop but also because the gas and water fluxes change along the channel length. Depending on the load, the flow regime inside the minichannels may vary between surface tension controlled slug flow and inertia controlled annular flow. He argued that it is desired to operate the fuel cell in the annular or dispersed
droplet flow regime since it provides a path for reactant flow in the presence of water. However, at part load of the fuel cell stack the flow regime is likely to change to slug flow.

Zhang et al. (2006) experimentally studied water transport and removal from the gas diffusion layer (GDL) and gas channel of a transparent fuel cell. The effects of cathode air flow rate on the liquid water distribution and cell performance were studied. At low air flow rates capillary wicking of the liquid water occurred from the GDL to the channel walls whereas at high air flow rates small droplets were swept way from the GDL surface. However, low gas velocities and high water production rate resulted in annular film/slug flow that caused occasional channel clogging.

In the slug flow regime, water droplets may grow large enough to randomly block the parallel channel passages that are connected by a common header. This can cause unwanted pressure drop and uneven flow distribution of air to the GDM surface that can lead to uneven current generation in the fuel cell. It is important that the water droplets forming on the surface of the gas diffusion media due to reaction in the fuel cell be removed quickly by the air stream before they can grow large enough to block the channel cross-section. The growth of the liquid droplet and its subsequent detachment from the channel wall is believed to be influenced by the air flow rate, the water flow rate to the droplet and also the contact angle between the droplet and the GDM surface. The objective of the present study is to numerically simulate the interaction of a growing water droplet and air stream flowing over it inside a minichannel for different values of air flow rate, water flow rate and contact angle at the droplet base.

**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>wall area</td>
</tr>
<tr>
<td>CA</td>
<td>contact angle</td>
</tr>
<tr>
<td>ACA</td>
<td>advancing contact angle</td>
</tr>
<tr>
<td>RCA</td>
<td>receding contact angle</td>
</tr>
<tr>
<td>d</td>
<td>grid spacing</td>
</tr>
<tr>
<td>g</td>
<td>gravity vector</td>
</tr>
<tr>
<td>H</td>
<td>Heaviside function</td>
</tr>
<tr>
<td>l_0</td>
<td>length scale</td>
</tr>
<tr>
<td>ms</td>
<td>milliseconds</td>
</tr>
<tr>
<td>p</td>
<td>pressure</td>
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<tr>
<td>t</td>
<td>time</td>
</tr>
<tr>
<td>t_0</td>
<td>time scale</td>
</tr>
<tr>
<td>u</td>
<td>x direction velocity</td>
</tr>
<tr>
<td>u_0</td>
<td>velocity scale</td>
</tr>
<tr>
<td>v</td>
<td>y direction velocity</td>
</tr>
<tr>
<td>V_{air}</td>
<td>air velocity at channel inlet</td>
</tr>
<tr>
<td>V_{liq}</td>
<td>liquid velocity at droplet base</td>
</tr>
<tr>
<td>w</td>
<td>z direction velocity</td>
</tr>
<tr>
<td>x</td>
<td>distance in x direction</td>
</tr>
<tr>
<td>y</td>
<td>distance in y direction</td>
</tr>
<tr>
<td>z</td>
<td>distance in z direction</td>
</tr>
<tr>
<td>κ</td>
<td>interfacial curvature</td>
</tr>
</tbody>
</table>

**Subscripts**

- in: inlet
- l: liquid
- x: \( \partial / \partial x \)
- y: \( \partial / \partial y \)
- z: \( \partial / \partial z \)

**Superscripts**

- *: non-dimensional quantity
- \( \rightarrow \): vector quantity

**NUMERICAL MODEL**

**Computational Domain**

Figure 1 shows the typical computational domain. The domain is 1.98x0.99x0.99 non-dimensional units in size. Cartesian coordinates are used with uniform grid.

![Computational domain](image)

Fig 1 – Computational domain

The air enters the domain at \( x^* = 0 \) and leaves the domain at \( x^* = 1.99 \). To take advantage of symmetry and reduce computation time, a water droplet is placed at the top wall equidistant from the walls in the x-y planes.

The number of computational cells in the domain is 256x128x64, i.e. 128 grids are used per 0.99\( l_0 \) where \( l_0 \) is 1 mm. This grid size is chosen to minimize numerical error and optimize computation time. Variable time step is used which is in the order of 1e-3.

\[ \mu \quad \text{dynamic viscosity} \]
\[ \nu \quad \text{kinematic viscosity} \]
\[ \rho \quad \text{density} \]
\[ \sigma \quad \text{surface tension} \]
\[ \tau \quad \text{time period} \]
\[ \phi \quad \text{level set function} \]
\[ \varphi \quad \text{contact angle} \]
Method
The complete incompressible Navier-Stokes equations are solved using the SIMPLER method [Patankar, 1980], which stands for Semi-Implicit Method for Pressure-Linked Equations Revised. The continuity equation is turned into an equation for the pressure correction. A pressure field is extracted from the given velocity field. At each iteration, the velocities are corrected using velocity-correction formulas. The computations proceed to convergence via a series of continuity satisfying velocity fields. The algebraic equations are solved using the line-by-line technique, which uses TDMA (Tri-Diagonal Matrix Algorithm) as the basic unit. The speed of convergence of the line-by-line technique is further increased by supplementing it with the block-correction procedure [Patankar, 1981].

Sussman et al. (1994) developed a level set approach where the interface was captured implicitly as the zero level set of a smooth function. The level set function was typically a smooth function, denoted as $\phi$. This formulation eliminated the problems of adding/subtracting points to a moving grid and automatically took care of merging and breaking of the interface. Furthermore, the level set formulation generalized easily to three dimensions. The present analysis is done using this level set technique.

The liquid vapor interface is identified as the zero level set of a smooth distance function $\phi$. The level set function $\phi$ is negative inside the bubble and positive outside the bubble. The interface is located by solving the level set equation. A fifth order WENO (Weighted, Essentially Non-Oscillatory) scheme is used for left sided and right sided discretization of $\phi$ [Fedkiw et al., 1998]. While $\phi$ is initially a distance function, it will not remain so after solving the level set equation. Maintaining $\phi$ as a distance function is essential for providing the interface with a width fixed in time. This is achieved by reinitialization of $\phi$. A modification of Godunov's method is used to determine the upwind directions. The reinitialization equation is solved in fictitious time after each fully complete time step. With $\Delta \tau = \frac{d}{2u_0}$, ten $\tau$ steps are taken with a third order TVD (Total Variation Diminishing) Runge Kutta method.

Governing Equations
Momentum equation -
\[
\rho \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\nabla p + \rho \vec{g} - \sigma \kappa \nabla H
\]
\[+ \nabla \mu \nabla \vec{u} + \nabla \mu \nabla \vec{u}^T \tag{1}\]
Continuity equation -
\[
\nabla \cdot \vec{u} = 0 \tag{2}\]

The curvature of the interface -
\[
\kappa(\phi) = \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{3}\]

To prevent instabilities at the interface, the density and viscosity are defined as -
\[
\rho = \rho_v + (\rho_l - \rho_v)H \tag{4}\]
\[
\mu = \mu_v + (\mu_l - \mu_v)H \tag{5}\]
$H$ is the Heaviside function given by -
\[
H = 1 \text{ if } \phi \geq 1.5d
\]
\[
H = 0 \text{ if } \phi \leq -1.5d
\]
\[
H = 0.5 + \phi/(3d) + \sin[2\pi\phi/(3d)]/(2\pi) \text{ if } |\phi| \leq 1.5d \tag{6}\]
where $d$ is the grid spacing.

The level set equation is solved as -
\[
\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0 \tag{7}\]

After every time step the level-set function $\phi$, is reinitialized as-
\[
\frac{\partial \phi}{\partial t} = S(\phi_0)(1-|\nabla \phi|)u_0 \tag{8}\]
\[
\phi(x,0) = \phi_0(x)
\]
$S$ is the sign function which is calculated as -
\[
S(\phi_0) = \frac{\phi_0}{\sqrt{\phi_0^2 + d^2}} \tag{9}\]

Initial Conditions
The liquid drop is placed in the domain at $x^* = 0.99$, $y^* = 0.99$ and $z^* = 0$, with $0.1l_0$ radius as shown in Fig. 1. All velocities in the internal grid points are set to zero. All physical properties are taken at $60^\circ$ C, 1 atm. The advancing and receding contact angles at the walls are specified as $140^\circ$ and $50^\circ$ respectively, which are obtained from the experimental data of Borelli et al. (2005). The gravity acts in the negative y direction.

Boundary Conditions
The boundary conditions are as following –
\[\text{• At the inlet (} x^* = 0 \text{)} :- \]
\[u = V_{air}; v = w = 0; \phi_e = 0 \tag{10}\]
\[\text{• At the outlet (} x^* = 1.98 \text{)} :- \]
\[u_e = v_e = w_e = 0; \phi_e = 0 \tag{11}\]
• At the plane of symmetry (z* = 0):
  \[ u_z = v_z = w = 0; \phi_z = 0 \]  \hspace{1cm} (12)

• At the bottom wall (y* = 0):
  \[ u = v = w = 0; \phi_y = -\cos\phi \]  \hspace{1cm} (13)

  where \( \phi \) is the contact angle.

• At the top wall (y* = 0.99):
  \[ u = w = 0; \phi_y = -\cos\phi \]  \hspace{1cm} (14)

  \[ v = V_{\text{liq}} \text{ if } \phi > 0; \]
  \[ v = 0 \text{ if } \phi \leq 0; \]

• At the wall (z* = 0.495):
  \[ u = v = w = 0; \phi_z = -\cos\phi \]  \hspace{1cm} (15)

Different values of advancing and receding contact angles have been specified at the leading and trailing edges of the droplet. The distance between the leading and trailing edges of the droplet is used to linearly interpolate the contact angle along the contact line between the droplet and the top wall.

**RESULTS AND DISCUSSION**

Figure 2 shows the droplets just before departure for different values of channel inlet air velocities. The air velocities used are obtained from the experimental data of Borelli et al. (2005). The receding and advancing contact angles are 50° and 140° respectively. The liquid inlet velocity is 0.132 m/s. Thus, the volumetric liquid flow to the drop increases or decreases as the base diameter increases or decreases. The air is blowing over the drop from left to right and pushes the drop forward and hence the drops are tilted towards the right. The droplets depart when the base pinches off.

Figure 3 shows the velocity field around the drop for the \( V_{\text{air}} = 0.71 \) m/s case in Fig. 2. The velocity vectors are plotted at the central x-y plane through the drop and the reference vector is shown in the upper right corner. The incoming air gets deflected by the hanging drop, changes direction and flows around the drop.
Figure 4 shows the droplet shapes for different values of incoming water velocities to the drop. The $V_{\text{air}}$ for all the cases is 0.71 m/s. The receding and advancing contact angles are $50^\circ$ and $140^\circ$ respectively. The droplet grows bigger with increase in the water flow rate. At the highest water velocity of 0.16 m/s, the drop does not depart from the channel wall with the droplet height increasing continually.

Figure 6 shows the effect of contact angles on the droplets. At low values of contact angles, RCA – $50^\circ$ and ACA – $95^\circ$ the droplet does not depart but continues to spread along the surface forming a liquid layer. At high values of contact angles, RCA – $95^\circ$ and ACA – $140^\circ$, the droplet departs almost immediately with much smaller departure diameter.

Table 1 lists the departure diameters in millimeters for all the cases presented above. The droplet departure diameter increase slightly with increase in $V_{\text{air}}$. This indicates that the air is exerting a force on the droplet opposite to the gravity which increases with increase in air flow rate thereby delaying the droplet departure. The droplet departure diameter is found to increase slightly with increase in incoming liquid velocity from 0.1 m/s to 0.13 m/s. However, at 0.16 m/s the droplet does not depart from the surface and continues to grow.

<table>
<thead>
<tr>
<th>$V_{\text{air}}$ (m/s)</th>
<th>$0.47$</th>
<th>$0.71$</th>
<th>$0.95$</th>
</tr>
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<tbody>
<tr>
<td>$(V_{\text{liq}} = 0.13 \text{ m/s},$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RCA – $50^\circ$,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ACA – $140^\circ$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$0.165$</td>
<td>$0.17$</td>
<td>$0.19$</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>$V_{\text{liq}}$ (m/s)</th>
<th>$0.1$</th>
<th>$0.13$</th>
<th>$0.16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(V_{\text{air}} = 0.71 \text{ m/s},$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RCA – $50^\circ$,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ACA – $140^\circ$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$0.155$</td>
<td>$0.17$</td>
<td>$-$</td>
<td></td>
</tr>
</tbody>
</table>

| Contact Angle | RCA – $50$,  | RCA – $50$,  | RCA – $95$,  |
|---------------| ACA – $95$ | ACA – $140$ | ACA – $140$ |
| $(V_{\text{air}} = 0.71 \text{ m/s},$ |        |        |        |
| $V_{\text{liq}} = 0.13 \text{ m/s})$ |        |        |        |
| $-$             | $0.17$  | $0.09$ |        |
The droplet departure diameter is found to decrease with increase in contact angle or decrease in surface wettability. At the lowest values of contact angle investigated the droplet did not depart but formed a liquid layer on the channel wall.

Thus, it is seen that at low values of contact angle and high water flow rates, the droplet may grow continually without departing and can possibly result in annular/slug flow. The mechanism of liquid transport to the droplet from the GDL and its surface wettability are the key parameters that can delay the droplet departure and needs to be investigated further.

CONCLUSIONS
1. Numerical simulation is carried out for a growing water droplet inside a minichannel with air flowing over the droplet.
2. At high liquid flow rates the droplet did not depart and the droplet diameter kept increasing continually.
3. The droplet departure diameter decreased with increase in contact angle at the channel wall. For the lowest values of contact angle the droplet did not depart but kept continually spreading on the wall. Such hydrophilic behavior is not desirable in fuel cell applications.
4. The mechanism of water transport to the droplet base from the GDM and its surface wettability are the key parameters that affect droplet departure. Future work is recommended in this area.

ACKNOWLEDGMENTS
The work was conducted in the Thermal Analysis and Microfluidics Laboratory at RIT.

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