COMPACT MODEL OF SLUG FLOW IN MICROCHANNELS

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ABSTRACT
This paper presents a theoretical investigation of the movement of liquid droplets and slugs in hydrophobic microchannels and develops a compact model for this type of two-phase flow. This model is used in the prediction of pressure drop and liquid water coverage ratio, key parameters in the operation of Proton Exchange Membrane Fuel Cells (PEMFC), the primary motivation for this work. A semi-empirical, periodic-steady two-phase separated flow compact model is formulated to characterize the slug flow behavior. The momentum equation includes the effects of acceleration, friction and surface tension on the pressure drop. The model considers spatial changes in slug velocity through the use of a force balance formulation. The model uses a departure scheme that computes slug size and shape at entrainment. The steady state slug flow compact model is capable of predicting liquid water coverage ratio and pressure drop using liquid and gas flow rates and advancing/receding triple point contact angles as its only inputs. The results indicate that the pressure drop increases as the droplet formation frequency increases.

INTRODUCTION
One of the key issues in operating a PEMFC is water management at the cathode to prevent oxygen starvation due to water clogging of the Gas Diffusion Layer (GDL) while maintaining proper hydration of the polymer membrane [1]. The use of microchannels for reactant transport brings about improved PEMFC performance [2], but more importantly, it makes portable fuel cells feasible. Thus, it is important to understand water transport in microchannels.

Liquid water is formed at the cathode and goes through the GDL, hydrophobic porous medium, and into the microchannel air stream. As water accumulates on the GDL surface it is entrained into the microchannel by the air and evacuated through the outlet. The flow patterns that develop vary depending on the flow conditions of the air, liquid water, and channel characteristics such as the aspect ratio and surface features [3]. Under certain conditions the water attaches to the wall and flows in the streamwise direction in an intermittent pattern. Such a flow pattern is called slug flow. This flow pattern is typically observed in hydrophobic microchannels. More specifically, pancake shaped slugs are observed in high aspect ratio microchannels, while spherical shaped slugs or deformed droplets are prevalent only in low aspect ratio microchannels.

Despite its importance, very few studies have been carried out on the water transport phenomena in air microchannels with distributed water entrainment. The challenges associated with the analysis of these flow patterns become compounded when water transport through the porous GDL is considered. This particular study focuses on the slug flow phenomena in hydrophobic microchannels. Several researchers have previously carried out studies on the slug flow pattern. Taitel and Barnea studied the slug flow theoretically and experimentally [4], while Zhang et al. improved the theoretical background of the slug flow by considering the pressure drop over the film zone [5].

However, the slug flow in their study differed technically from the slug flow of the present study in that they dealt with an intermittent flow of elongated bubbles that had a very thin surrounding film of liquid. In this study we concentrate on the specific case of slug flow in a high aspect ratio hydrophobic microchannel with a single side injection slot, where the pancake shaped slugs are prevalent.

The objective of this study is to develop a one-dimensional compact model based on experimental observations, thereby capturing the physics behind the slug flow. Since the liquid phase exists as a discontinuous slug and has a different velocity from the gas phase, complete analytical models are very complex and difficult to solve. However, a steady-state model can be derived with the assumption that the liquid slug is periodic.

The momentum equation in the slug flow compact model consists of the effects of acceleration, friction, and surface tension on pressure drop, and accounts for spatial changes in slug velocity through the use of a force balance formulation. In
addition, the model is fully encompassing by employing a departure scheme that calculates slug size and shape at entrainment. As a result, the model predicts liquid water coverage ratio and pressure drop using liquid and gas flow rates and advancing/receding contact angles as its only inputs.

**NOMENCLATURE**

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<td>( A )</td>
<td>liquid wall contact surface area</td>
<td>( \text{m}^2 )</td>
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<tr>
<td>( A_{ch} )</td>
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<td>( A_p )</td>
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**Greek Symbols**

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<th>Symbol</th>
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</tr>
<tr>
<td>( \theta_r )</td>
<td>receding contact angle</td>
<td>rad</td>
</tr>
<tr>
<td>( \theta_s )</td>
<td>advancing contact angle</td>
<td>rad</td>
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**Subscripts**

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<td>( i )</td>
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</tr>
<tr>
<td>( s )</td>
<td>slug</td>
</tr>
<tr>
<td>( t )</td>
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**STEADY-STATE SLUG FLOW MODELING**

Figure 1 illustrates the schematic of the slug flow in the microchannel geometry considered in this study. The intermittent liquid droplet attached to the side wall is driven by the gas along the channel, which is in axial (e.g. \( z \)-axis) direction. The slug flow model is divided into two regions: the slug region with a length of \( l_s \) and the gas-phase region with length \( l_g \). Note that \( l_s \) is a unit cell length. The air moves at \( U_g \) while the liquid slug moves at \( U_s \).

The governing equations are developed for both the liquid and gas-phase in both the slug and gas only region by applying the momentum balance to a fixed control volume encompassing each phase. The following assumptions are made for the present model:

1. The slug flow is periodic-steady.
2. The slug flow is laminar, fully-developed and is driven by pressure.
3. There is no or negligible liquid film on the wall.
4. The flow is isothermal, and there are no Marangoni effects.
5. There is no mass transfer at the gas-liquid interface.
6. Gravity is negligible since the Bond number is very small.
7. Gas properties are averaged at each cross section along the axis of the channel, thereby varying only in the direction of the flow.
8. The difference in surface properties between the channel wall and the GDL are not considered.
9. The shear stress coefficient is constant along the channel periphery.

The local pressure \( P \) is calculated by considering the gas flow phase momentum force balance. However, the governing equations for the liquid phase in the slug region are also derived to corroborate validity. Based on the periodic steady-state assumption, the average pressure drop at any axial microchannel location is given by:

\[
\frac{dP}{dz} = \frac{l_s}{l_s} \frac{dP}{dz} \bigg|_{g} - \frac{l_g}{l_s} \frac{dP}{dz} \bigg|_{s} \frac{dP}{dz} \bigg|_{\text{min}} \bigg|_{\text{loss}}
\]  

(1)

Even under global steady-state conditions, at any given axial microchannel location there is an inherent “transient” due to the cyclical passing of slugs through that point. Thus, when calculating the time averaged pressure drop in the numerical scheme, the flow is considered steady with the pressure drop per grid given by Eq. (1).
The governing equations for the pressure drop for each phase in each region are given as follows:

**Gas-phase region:**

\[
\frac{dP}{dz} = \frac{d}{dz} \left[ \rho_g U_g^2 + \frac{\tau_{gW}}{A_{gh}} \right] \\
= \frac{d}{dz} \left[ \rho_g U_g^2 \right] + C_{fW} \frac{\rho_g U_g^2}{2A_{gh}} 
\]

(2)

**Slug region:**

**Gas phase**

\[
\frac{dP}{dz} = \frac{1}{\alpha} \frac{d}{dz} \left( \rho_g U_g^2 \alpha \right) + \frac{\tau_{gW}}{\alpha A_{gh}} + \frac{\tau_{gW}}{\alpha A_{gh}} 
\]

(3)

**Liquid phase**

\[
\frac{dP}{dz} = \frac{1}{1-\alpha} \frac{d}{dz} \left( \rho_s U_s^2 (1-\alpha) \right) \\
+ \frac{\tau_{sl} P_{sl}}{(1-\alpha) A_{gh}} - \frac{\tau_{lW}}{(1-\alpha) A_{gh}} \\
+ \sigma p_{surf} \frac{(\cos \theta_r - \cos \theta_a)}{(1-\alpha) l_s A_{gh}} 
\]

(4)

**Whole slug region**

\[
\frac{dP}{dz} = -\alpha \frac{dP}{dz} - (1-\alpha) \frac{dP}{dz} \\
= \frac{d}{dz} \left( \rho U_s^2 (1-\alpha) + \rho_s U_s^2 \alpha \right) \\
+ \frac{\tau_{sl} P_{sl}}{A_{gh}} + \frac{\tau_{gW} P_{gW}}{A_{gh}} \\
+ \frac{\sigma p_{surf} (\cos \theta_r - \cos \theta_a)}{l_s A_{gh}} 
\]

(5)

where \( \rho_g \) and \( \rho_s \) are the densities of air and liquid water, respectively, and \( A_{gh} \) is the cross-sectional area of the channel. The local velocity of the air is given by \( U_g \), and \( U_s \) is the velocity of the liquid slug. The wall shear stress is denoted by \( \tau_{gW} \) and \( \tau_{sl} \) for the gas-wall and liquid slug-wall interfaces, respectively. The cross-sectional void fraction is given by \( \alpha \), while \( \theta_r \) represents the receding contact angle and \( \theta_a \) the advancing contact angle. The water surface tension coefficient is denoted by \( \sigma \). \( p_{surf} \) is the wall-gas perimeter, \( P_{sl} \) is the liquid-gas contact area, and \( P_{surf} \) the slug contact line length. Note that the governing momentum equations for each phase in the slug region are unified in Eq. (5).

As can be seen from Eqs. (2)-(4) the governing momentum equations account for acceleration pressure drops. However, for most cases in this study, the Mach numbers are very small and these terms can therefore be neglected. It should be noted, however, that for certain upstream flow conditions (high pressure and air flow rate) the flow can accelerate quite fast as it tends toward choking conditions (Rayleigh Flow) in which case the acceleration pressure terms must be taken into account. Note that the governing momentum equation for the liquid phase in the slug region includes surface tension effects. The surface tension induced pressure drop is given by the slug length and contact angles. Note also that the surface tension induced pressure gradient includes only triple points contact line effects. The two-phase liquid-gas surface tension is exactly balanced by the pressure jump across the interface, thereby canceling each other out in the slug region.

It is necessary to define shear stresses from 1D variables for the purpose of well-posing the governing equations. Based on the fully developed flow assumptions, developing effects can be neglected and relationships for the friction coefficients and wall shear stresses can be established as a function of the aspect ratio. Wall shear stresses and friction coefficient are expressed as

\[
\tau_{gW} = \frac{1}{2} C_{fW} \rho_g U_g^2 
\]

(6)

\[
\tau_{sl} = \frac{1}{2} C_{fsl} \rho_s U_s^2 
\]

(7)

\[
C_{fsl,Re} = 24(1-1.3553\beta + 1.9467\beta^2 - 1.7012\beta^3 + 0.9564\beta^4 - 0.2537\beta^5) 
\]

[6](8)

where \( C_f \) indicates the friction coefficient, \( \beta \) the aspect ratio, \( Re \) is the Reynolds number, index \( k \) is \( wg \) or \( sl \), subscript \( wg \) denotes the wall-gas interface, and subscript \( sl \) the wall-liquid interface.

Careful attention should be paid to the interfacial shear stresses. From the viewpoint of the gas flow, the liquid interface acts like a wall. Therefore, a friction coefficient corresponding to the gas flow against the wall is used to calculate the interfacial shear stress [7]. An important consideration is the relative slug to gas velocity. The following assumptions are made regarding the movement of the slug:

(10) The slug shape is simplified as a rectangular parallelepiped.

(11) The slug velocity is the velocity at the center of inertia of the slug.

(12) The slug velocity is small relative to the gas velocity.

(13) Possible differences in velocity between the front and the back end of the slug are not significant. In other words, slug deformations, such as elongation and contraction, are ignored.

(14) The receding and advancing contact angles are assumed to be constant. That is, contact angle hysteresis is constant and independent of flow variables, such as slug velocity.

(15) The separation between slugs is relatively large compared to the length of slug.

The slug flow model considers pancake shaped slugs prevalent in high aspect ratio hydrophobic microchannels. Furthermore, the model simplifies the slug shape as given in assumption (9) for the sake of simplicity. Corresponding to assumption (11), the interfacial velocity is assumed to be \( 2U_s \) [8]. As a result, the interfacial shear stress is given by: 

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\[
\tau_i = \frac{1}{2} C_{f,i} \rho_g (U_g - U_i)^2 \]
\[
\approx \frac{1}{2} C_{f,i} \rho_g (U_g - 2U_i)^2
\]

where \( C_{f,i} = C_{f,loc} \)

The wall shear coefficients do not include secondary flow effects arising from circulation around the slug. Instead, these effects are included in the minor head loss term in Eq. (1) to account for the sudden contraction pressure loss and sudden expansion pressure recovery induced by the slug geometry. They are derived from the Bernoulli equation. Figure 2 illustrates the notation and geometry used for computation of the minor head losses. The minor head losses are computed as follows:

**Sudden contraction pressure loss**

\[
\Delta P = \frac{\rho V_i^2}{2} - \frac{\rho V_f^2}{2} + K \frac{\rho V_f^2}{2},
\]

\[
K_w \approx 0.42 \left(1 - \frac{A_f}{A_i}\right) \text{ valid up to } \alpha \approx 0.6
\]

**Sudden expansion pressure recovery**

\[
\Delta P = \frac{\rho V_f^2}{2} - \frac{\rho V_i^2}{2} + K \frac{\rho V_i^2}{2}, \quad K = \left(1 - \frac{A_i}{A_f}\right)
\]

The value of \( K_{wc} \) is that corresponding to a minimum diameter sudden contraction (\textit{i.e. vena contracta}). The sudden expansion equation is derived by using a well known control volume analysis [9]. In practice, the actual value of the minor head losses is dependent on the shape of the slug. In the present calculations the simplest structure, a rectangular parallelepiped with sharp edges, yields an upper bound of the minor head losses.

![Figure 2: Geometry used in estimation of minor head losses (\( \Delta P_c \) indicates sudden contraction pressure loss and \( \Delta P_s \) sudden expansion pressure recovery)](image)

In the governing equations for slug flow, even if the shear stresses and the minor head losses are defined, local slug velocity \( U_i \) as well as geometric variables such as void fraction \( \alpha \), slug length \( l_s \), gas-phase region length \( l_{gr} \), advancing contact angle \( \theta_a \), and receding contact angle \( \theta_r \), are still unknown. To close the model, a formulation for local slug velocity must be introduced and the slug geometric variables should be established. The local slug velocity \( U_i \) can be obtained from a force balance on the liquid slug, on the assumption that the receding and advancing contact angles remain constant, as per assumption (13). The focus of this model is in the global physics and behavior of the slug flow under periodic, steady-state conditions.

In order to determine local slug velocity \( U_i \), four representative forces are considered in the force balance [10]. These forces on the slug are categorized as drag forces and resistive forces. The former consists of pressure induced form drag and viscous shear friction drag due to interfacial shear stress. The latter is the liquid wall friction and the surface tension force. Figure 3 illustrates the schematic for the entire force balance. \( F_p \) denotes the pressure induced form drag force, \( F_s \) the viscous shear friction force, \( F_w \) the liquid wall friction force, and \( F_i \) the surface tension force.

![Figure 3: Force balance on a liquid slug in microchannels](image)

The force balance is expressed as

\[
M \frac{dU_i}{dt} = F_p + F_s - F_w - F_i
\]

where \( M \) is the slug mass, and \( t \) the time. Formulations for each force are established as follows.

The pressure force is given by

\[
F_p = \int_{\Omega} P \cdot n_z \, d\Omega \approx A_f \left(1 - \frac{A_i}{A_f}\right) \int_{l_{gr}} \frac{dP}{dz} \, dz
\]

where \( n_z \) is a unit vector in the \( z \) direction, \( \Omega \) the slug surface, \( A_f \) the projected area of slug in the \( z \) direction, and the integral on the right hand side accounts for the gas phase pressure drop in the slug region. Note that the pressure force on the slug is due to the gas phase pressure drop in the slug region.

The viscous force is given by

\[
F_s = \int_{\Omega} \frac{C_{f,i}}{2} \rho_g (U_g - U_i)^2 \, d\Omega
\]

\[
\approx \frac{C_{f,i}}{2} \rho_g (U_g - 2U_i)^2 A_i
\]

where \( \Omega \) is the interfacial surface between the liquid and gas, \( U_i \) is the interfacial velocity, \( A_i \) is the interfacial area and \( C_{f,i} \) is the interfacial friction coefficient. Note that the friction coefficient for the gas flow against the wall is used as the interfacial friction coefficient as mentioned above.

The surface tension force is given by

\[
F_i = \int_c n_z \, dl \approx \frac{1}{4} C_s \rho_{surf} (\cos \theta_i - \cos \theta_c)\]

\[
C_s = \frac{58}{\theta_e + 5} + 0.14
\]

where \( C \) is the liquid-gas-wall line contact contour, \( \sigma \) the liquid-gas surface tension coefficient, \( n_z \) a unit vector normal to \( C \) but tangent to \( z \), \( dl \) a length increment along the curve \( C, \rho_{surf} \) the surface tension contact line, and \( \theta_e \) the equilibrium contact angle. For the surface tension force coefficient, \( C_s \), the Alhayes and Winterton’s correlation [11] is employed. The
surface tension coefficient is a formulation to account for deformations related to contact angle hysteresis effects based on equilibrium contact angle. Although this correlation is derived for bubbles in liquid flows, we adopt this correlation since the phases in questions are the same, only in reverse. In addition, the contact angle hysteresis is inherently included in the formulation for the surface tension force through the advancing and receding contact angles.

The liquid wall friction force is given by

\[ F_w = \int_A \tau_{wl} dA, \quad \tau_{wl} = C_{f,wl} \frac{\rho U_s^2}{2} \]  

(16)

where \( \tau_{wl} \) is the liquid-wall shear stress, and \( A \) is the liquid-wall contact surface area. For the liquid-wall shear stress, the fully developed flow condition inside the slug is also assumed.

Once the characteristic forces are defined, the local slug velocity can be obtained from the force balance. The local slug velocity is then plugged into the interfacial friction term of the momentum governing equation for the gas phase in the slug region. In actual numerical computations, iterations between the momentum governing equation and the force balance equation are required due to the coupling of the pressure drop and slug/gas velocities in the slug region. First the pressure drop in the gas phase for the slug region is assumed. Then the slug velocity as a function of time is calculated through the force balance. The position of the slug as a function of time is determined by integrating the time dependent slug velocity. Then the pressure drop in the gas phase for the slug region is assumed. This integration is carried out numerically using the trapezoidal rule, an approach adopted from Glockner et al. [12]. The slug velocity is determined by the force balance with the assumed pressure drop in the gas phase for the slug region (i.e., the assumed pressure force). This calculated slug velocity is then used to compute the pressure drop from the momentum equation. This procedure is repeated until the pressure drop and the slug velocity have converged.

Even though the slug velocity can be determined from the force balance, slug geometric variables are still unknown. By simplifying the pancake shaped slug as a rectangular parallelepiped shape, the unknown geometric variables are reduced to \( \alpha, l_s, l_g, \theta_s \), and \( \theta_g \) as in Figure 4, which shows a slug in a 500 \( \mu \)m width (\( W_{ch} \)) and 45 \( \mu \)m depth (\( H_{ch} \)) hydrophobic channel with 20 \( \mu \)m width (\( l_{slot} \)) and a 45 \( \mu \)m depth side injection hole. Since contact angles averaged along the channel length are determined from experimental observations, the unknown geometrical variables are further reduced to three: \( \alpha, l_s \), and \( l_g \).

Therefore, the departure scheme consists of three equations to solve for these three unknowns: (1) the correlation between slug length \( l_s \), and void fraction \( \alpha \), (2) liquid mass conservation, and (3) the force balance for detachment criterion. The slug length-void fraction correlation underlies the physics behind slug shape as a function of water injection. This correlation can be regarded as the slug growth equation. The liquid mass conservation establishes a relationship between slug mass, velocity, period and water injection rate. It states that the liquid water injection rate is equal to the slug period times the volume of the slug. Finally, the force balance is used to determine slug size at detachment. The void fraction and slug length are determined by the slug growth and force balance equations, while the gas phase region length is obtained through the mass conservation equation. This last statement can be summarized and mathematically expressed as follows:

The correlation between void fraction and slug length:

\[ \alpha^2 L_c \approx 20(1-\alpha)^2 W_{ch} \left( \frac{\rho_s U_s^2 D_{ch}}{\sigma} \right)^{0.4} \left( \frac{m_s}{m_g} \right)^{0.2} \]  

(17)

Mass balance:

\[ Q = U_s (1-\alpha) A_{ch} \frac{L}{L_s + L_g} \]  

(18)

Period:

\[ T = \frac{(1-\alpha) A_{ch} L_s}{Q} \]  

(19)

where \( Q \) is the water injection flow rate, \( T \) the detachment period, \( l_{slot} \) the water injection slot width, \( H_{ch} \) the depth of the channel, and \( W_{ch} \) the width of the channel.

![Figure 5: Layout of the U-shaped microchannel](image)

The slug growth equation is derived from experimental data. The data is from experiments conducted on U-shaped hydrophobic microchannels (Hidrovo et al. [13]) as per Figure 5. In U-shaped microchannels, the air is blowing from the gas inlet to outlet, while the water is injected through the water inlet. These samples are microfabricated on a silicon wafer substrate with an anodically bonded glass cover that enables visualization. The samples are rendered hydrophobic through molecular vapor deposition (MVD) of FTDS self assembled monolayers (SAMs), a process performed by Applied Micro Structures, Inc. (AMST). The measured values for the receding and advancing contact angles were 70° and 110°, respectively. Visualization was performed using a Nikon TE2000U inverted microscope.
epifluorescence microscope with a 4X objective and a Roper Scientific 12-bit CoolSNAP ES CCD camera.

The slug growth equation relating void fraction to slug length is derived by applying the II Theorem to the experimental data from the U-shaped hydrophobic microchannels. A critical assumption of the correlation is that the injected water completely fills the channel depth. This is a reasonable assumption since the channel depth is relatively small compared to the other dimensions in a high aspect ratio channel. The correlation reveals that as the liquid water injection rate increases, the slug length also increases as and the gas flow rate increases, the slug frequency goes up, which means the slug length decreases [13]. Note that the slug length is inversely proportional to Weber number in the correlation.

The force balance in the departure scheme employs the same formulae of representative forces as given by Eqs. (13) - (16). It is apparently seen that the slug is stationary before departure, yet the slug’s initial velocity is not zero so that the liquid wall friction force is added to the force balance in the departure scheme. The departure criterion requires for the drag force to be bigger than the reluctance force. Numerically, the force balance algorithm checks that criterion against the corresponding void fraction-slug length correlation to establish departure.

The mass balance is used to determine slug period after the void fraction and the slug length at departure have been established. The gas phase region length can then be determined from the slug period and length.

![Figure 6: Schematic of slug flow liquid water coverage](image)

The departure scheme is also useful in the determination of the liquid water coverage, an important parameter in the operation of PEMFC. Since the slug flow has temporal and spatial fluctuations due to the discontinuous liquid phase, careful considerations must be taken when deriving the liquid water coverage. The liquid water coverage only takes into account the GDL surface since this is the surface of importance in the transport of reactants to the catalyst sites. Figure 6 shows a schematic of the geometry used to calculate the liquid water coverage. The liquid water coverage is given as

\[
\text{Water Coverage} = \sum_{i=1}^{N} \left(1 - \alpha\right) \frac{W_{ch}}{L_s + L_g}
\]  

(20)

where \(W_{ch}\) is the height of channel and \(N\) the grid number. The liquid water coverage can be calculated as long as the void fraction, the slug length, and the gas phase region length are known.

Having established the analytical framework, the actual numerical algorithm used for computations is shown in Figure 7. The algorithm was written on FORTRAN 90 and is based on the finite volume method [14].

DISCUSSIONS

The understanding of the characteristics physics behind the slug flow is the main objective of this study. To this end, the effects of variable properties (e.g., gas density and viscosity), minor head losses, and pressure gradient variations are presented in this section. The slug geometry is kept fixed with specified values for better comparison between different flow conditions.

Variable properties and minor head losses effects are discussed first. Figure 8 shows the difference in pressure profile for constant versus variable properties along the channel in a 550 μm wide by 200 μm deep microchannel which is 30 mm in length. Note that in all the calculations from here, the water injection point (\(z=0\)) is located at the beginning of this long straight channel, so the whole channel becomes two-phase flow region, and the inlet pressure indicates the pressure at \(z=0\). The operating conditions in both cases are as follows: inlet pressure 2 atm, temperature 296.5K (isothermal conditions), superficial gas velocity \(j_f\) 17.48 m/s, superficial liquid velocity \(j_l\) 1.5 mm/s, receding contact angle 70°, and advancing contact angle 110°. The geometric variables associated with the slug are given as follows: slug length \(l_s=3\) mm, gas phase region length \(l_g=7\) mm and void fraction \(\alpha=0.6\). As can be seen from Figure 8 the differences in pressure profile caused by the variable properties are not significant in this case: the pressure drop for the variable properties case is 5.52 kPa, while the constant properties case pressure drop is 5.38 kPa.

![Figure 8: Local pressure along the channel calculated by constant and variable properties](image)  

![Figure 9: Effect of Minor head losses on local pressure prediction](image)
or head losses we now focus our attention to the liquid slug region, calculated from Eq. (5), as a function of microchannel position for the same operating conditions as in the previous cases. Note that the pressure gradient variation is focused only on the slug region, because the pressure gradient variation in the gas-phase only region is insignificant in microchannels. Figure 11 (b) shows the friction and acceleration contributions to the total pressure gradient in the slug region. The acceleration pressure gradient has two components: liquid phase acceleration and gas phase acceleration. Note that the pressure gradient induced by the surface tension is constant due to the non-variable slug geometry. From Figure 11 (a) it is apparent that the total pressure gradient decreases at the beginning microchannel, just after slug entrainment, reaching a minimum and then increasing along the microchannel. The reason behind this behavior becomes apparent by looking at Figure 11 (b) and Eq. (5). The friction pressure gradient is caused by the liquid wall friction and the gas wall friction, and is therefore proportional to their velocity. Since the liquid water properties, such as density and viscosity, are larger relative to air, the friction pressure gradient is mainly dependent on slug velocity. As such, the frictional pressure gradient follows the same slug velocity pattern as a function of microchannel position, rapidly increasing at the beginning of the microchannel, just after slug entrainment, and then tending towards an asymptotic value. On the other hand the acceleration pressure gradient rapidly decreases at the beginning of the microchannel and then tends towards zero. Since the acceleration pressure gradient induced by the gas variable properties is very small, the behavior of the overall acceleration pressure gradient is mostly caused by the liquid phase acceleration. Based on the slug velocity profile from Figure 11, the acceleration of the slug rapidly decreases along the channel and then tends towards zero as the velocity plateaus towards its terminal value. This is the same pattern of the overall acceleration pressure gradient along the channel. Therefore, even if the friction pressure gradient is proportional to the slug velocity, the total pressure gradient decreases at the beginning due to the sharp decrease of the acceleration pressure gradient of the liquid phase. However, whereas the acceleration pressure gradient is very small value downstream, the friction pressure gradient remains proportional to the slug velocity, causing an increase in the total pressure gradient.

Having considered the effects of variable properties and minor head losses we now focus our attention to the liquid slug velocity which is determined through the force balance. Figures 10 (a) and (b) show the slug velocity as a function of time and channel position, respectively. The operating conditions are the same as in the previous cases. It is apparent from these figures that the slug rapidly accelerates at the beginning of the microchannel just after detachment and then approaches a terminal velocity as it travels down the microchannel. Under these particular operating conditions the slug terminal velocity is 1.16 m/s, about 1/15 of the superficial gas velocity.

The fundamental slug flow physics can be better understood by looking at the pressure gradient along the channel. Figure 11 (a) depicts the total pressure gradient in the slug region, calculated from Eq.(5), as a function of microchannel position for the same operating conditions as in the previous cases. Note that the pressure gradient variation is focused only on the slug region, because the pressure gradient variation in the gas-phase only region is insignificant in microchannels. Figure 11 (b) shows the friction and acceleration contributions to the total pressure gradient in the slug region. The acceleration pressure gradient has two components: liquid phase acceleration and gas phase acceleration. Note that the pressure gradient induced by the surface tension is constant due to the non-variable slug geometry. From Figure 11 (a) it is apparent that the total pressure gradient decreases at the beginning microchannel, just after slug entrainment, reaching a minimum and then increasing along the microchannel. The reason behind this behavior becomes apparent by looking at Figure 11 (b) and Eq. (5). The friction pressure gradient is caused by the liquid wall friction and the gas wall friction, and is therefore proportional to their velocity. Since the liquid water properties, such as density and viscosity, are larger relative to air, the friction pressure gradient is mainly dependent on slug velocity. As such, the frictional pressure gradient follows the same slug velocity pattern as a function of microchannel position, rapidly increasing at the beginning of the microchannel, just after slug entrainment, and then tending towards an asymptotic value. On the other hand the acceleration pressure gradient rapidly decreases at the beginning of the microchannel and then tends towards zero. Since the acceleration pressure gradient induced by the gas variable properties is very small, the behavior of the overall acceleration pressure gradient is mostly caused by the liquid phase acceleration. Based on the slug velocity profile from Figure 11, the acceleration of the slug rapidly decreases along the channel and then tends towards zero as the velocity plateaus towards its terminal value. This is the same pattern of the overall acceleration pressure gradient along the channel. Therefore, even if the friction pressure gradient is proportional to the slug velocity, the total pressure gradient decreases at the beginning due to the sharp decrease of the acceleration pressure gradient of the liquid phase. However, whereas the acceleration pressure gradient is very small value downstream, the friction pressure gradient remains proportional to the slug velocity, causing an increase in the total pressure gradient.

As described in the modeling section, through the departure scheme this model is able to predict the local pressure and the water coverage ratio over the channel. Based on the empirical data from the U-shaped microchannel experiments, the force balance formulation in the departure scheme allows determination of the slug geometry in terms of the slug length and the void fraction (slug width). Figures 12 (a) and (b) show the comparison between the calculated slug length from the
departure scheme and the actual slug length measured from the U-shaped microchannel experimental data for the cases of 10 μl/min and 50 μl/min water injection rate, respectively. The microchannel dimensions are 500 μm width, 45 μm depth, and 10 μm slot width for 50 μl/min water injection rate and 50 μm slot width for 10 μl/min water injection rate, while the operating conditions are inlet pressure 2 atm, temperature 296.5K, receding contact angle 70°, and advancing contact angle 110°. As can be seen the agreement between model prediction and experimental results is generally good.

The calculated slug velocity as a function of microchannel position is shown in Figure 13. This velocity profile is different from the one in Figure 10 for several reasons. The operating conditions are the same as those used in the computation of Figure 10 except for the specified flow rates, which are 18.9 ml/min for the gas flow rate and 10 ml/min for the water injection rate. As such, the slug geometry is also different with the slug length being 337.8 μm and the void fraction 0.703. Just as in the case presented in Figure 10, the slug velocity keeps rapidly increases at the beginning of the microchannel, right after slug entrainment. However, unlike the case of Figure 10, the slug velocity depicted in Figure 13 does not reach a plateau or terminal velocity. Instead, it continues to accelerate as it moves down the microchannel, albeit at a much slower rate. These differences arise from the high aspect ratio of the channel (500 μm width and 45 μm depth for Figure 13 and 550 μm width and 200 μm depth for Figure 10) which results in a larger pressure drop and, more importantly, induce substantial gas compressibility and acceleration effects throughout the whole microchannel length. In addition, the smaller slug size and mass translate into larger acceleration. Figure 14 shows the Mach number variation along the microchannel. $Ma_G$ and $Ma_S$ denote the Mach number of the gas-phase region and the slug region, respectively. The slug Mach number increases rapidly at the downstream of the microchannel as a result of the higher pressure drop.

Figure 15 shows the liquid water coverage calculation. The microchannel geometry and operating conditions are the same as those used to calculate slug length and void fraction through the departure scheme. The water coverage calculation used the microchannel which is 7.7 mm long straight channel, and the water injection point is located at the inlet of the channel ($z=0$). The water coverage ratio decreases as the air mass flow rates increase and, as expected, it is proportional to the liquid water injection rate.

Finally, the microchannel pressure drops as a function of air flow rate for the two different water injection rates are shown in Figure 16. The operating and geometrical conditions are the same as those used to calculate the water coverage ratio. From Figure 16 it can be seen that the pressure drop is linearly proportional to the air mass flow rate. Similarly, the pressure drop also increases with liquid water injection rate. Since the slug frequency goes with the air flow rate in the departure scheme, it can be said that the pressure drop increases in proportion to the rise in the droplet formation frequency.

**CONCLUSIONS**

This study interprets slug flow using a new, compact numerical scheme and modeling. We first developed a periodic steady slug flow model that takes into account the discontinuous liquid phase and slug velocity. Furthermore, numerical schemes for the force balance, which determine slug velocity, and for the slug departure criterion are introduced for the first time.

Through this model, we have learned that the departure scheme and local slug velocity for a specified aspect ratio are critical factors in predicting the pressure drop and the liquid water coverage ratio in this type of flows. In addition, the overall pressure drop consists of acceleration, friction, induced surface tension, and minor head loss components. For the slug flow, minor head loss is one of the crucial components in the overall pressure drop.

In conclusion, even if the model does not cover the water transport physics through the GDL, this study not only make a better understanding of the physics behind the slug flow in the microchannel, but it also provides a solid foundation for solving the integrated issue encompassing the GDL and microchannels of PEMFC. Future research should be aimed at validating this model experimentally with the use of long straight single injection microchannels to better understand slug dynamics as well as verifying its velocity as a function of position in the microchannel.

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