A Semi–Empirical Model for Pressure Drop Prediction in the Anode Microchannel of a DMFC

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Abstract

In this paper, the pressure drop trend in the anode microchannel of a miniature direct methanol fuel cell is investigated. Due to the production of CO_2 gas in the fuel cell, the flow is considered to be two phase and also experiments have shown that the effect of pressure drop attributable to interfacial forces is significant. Several homogeneous and separated two phase flow models, some of them designed to consider surface tension effects, are compared with available experimental data and results suggest these models' incapability to even approximately predict the actual pressure drop. Therefore, a previously used semi-empirical model, based on a correlation between the pressure drop and the number of gas slugs, is modified to estimate the pressure drop in the microchannel more accurately. This work can be used to aid the design of fuel pumps and anode flow channels for miniature direct methanol fuel cell systems.

Keywords

μDMFC, Microchannel, Pressure Drop, Semi-Empirical Model, Two Phase Flow

Introduction

Miniature Direct Methanol Fuel Cells (μDMFCs) are considered to be the best alternative to replace conventional battery systems in portable electronic devices (laptops, cell phones, etc) due to their high energy density, safe fuel storage and transportation, relatively simple structure, and low environmental pollution [1]. However, in common passive DMFCs, environmental and operational conditions affect the cell performance significantly and therefore lead to some problems in mobile usages [2]. Utilizing a method to pump the fuel into the cell, active fuel delivery, have been shown to improve the performance of the system as well as lowering its dependability on operating conditions [3].

Estimating the pressure drop along the path of the fuel is one of the most important steps in selection and design of an efficient fuel delivery system for the μDMFC. In one of the first works on the pressure drop in anode of a DMFC, Argyropoulos et al. [4] employed a homogeneous model for two phase flow and concluded that pressure drop in the anode is a non-linear function of inlet methanol flow rate, but relatively invariant with current density. Later Yang et al. [5] experimentally investigated two phase flow pressure drop behavior in the anode flow field of a vertical DMFC with a single serpentine channel. They found that pressure drop exhibited a peak with increasing current density but monotonically increased with methanol solution flow rate. They also found that for high flow rates, the pressure drop acted almost independent of current density. In the both above mentioned works, it is important to note that capillary forces could be neglected. Recently, Buie et al. [6] focused on two phase pressure drop in μDMFC microchannels and used a novel experimental technique to measure two phase flow characteristics in order to derive an empirical correlation for pressure drop. Their results suggested that pressure drop was dominated by interfacial forces and it scaled with number of gas slugs, surface tension, and the diameter of the largest sphere inscribed in the channel.

In this study, in order to gain an elementary estimation, several two phase models—homogenous, separated flow, and also an intermittent bubble/slug flow—are used to calculate the two phase pressure drop of the flow in the anode of a μDMFC identical to the one used in Buie et al.'s [6] experiments, and also the models' results are compared to these experimental data. Due to the incapability of these general models to capture the actual trend of pressure drop, an empirical method suggested by Buie et al. [6] is modified using the data from his own experiments to predict the pressure drop behavior.

TABLE I: Homogeneous flow models used in this study

Model	Formula
McAdams et al. [8]	$\mu_{\mathrm{TP}} = \left(\frac{x}{\mu_g} + \frac{1-x}{\mu_l}\right)^{-1}$
Duckler et al. [9]	$\mu_{\mathrm{TP}} = \beta\mu_g + (1-\beta)\mu_l$
Beattie et al. [10]	$\mu_{\mathrm{TP}} = \beta\mu_g + (1-\beta)(1+2.5\beta)\mu_l$

Homogeneous Flow Models

A homogeneous flow model is the simplest two phase flow model; it treats two phase flow as a single phase flow with mixture properties. A two phase pressure drop consists of frictional, accelerational, and gravitational terms.

$$\left(\frac{dp}{dx}\right)_{\mathrm{TP}} = \left(\frac{dp}{dx}\right)_{\mathrm{fric}} + \left(\frac{dp}{dx}\right)_{\mathrm{acc}} + \left(\frac{dp}{dx}\right)_{\mathrm{gra}} \qquad (1)$$

In this study, the gravitational term is neglected, because the flow is horizontal, and the accelerational term is negligible because of the flow's very low Reynolds number. Thus, the total pressure drop is assumed to be approximately equal to frictional term, which can be defined:

$$\left(\frac{dp}{dx}\right)_{\mathrm{TP}} = \left(\frac{dp}{dx}\right)_{\mathrm{fric}} = \frac{2f_{\mathrm{TP}}G^2}{\rho_{\mathrm{TP}}D_h} \qquad (2)$$

where D_h, G and f_{TP}, are hydraulic diameter, mass flux and two phase friction factor respectively, and ρ_{TP} is two phase density:

$$\rho_{\mathrm{TP}} = \left(\frac{x}{\rho_g} + \frac{1-x}{\rho_l}\right)^{-1} \qquad (3)$$

The two phase friction factor can be expressed as an exponential function of the two phase Reynolds number:

$$f_{\mathrm{TP}} = N\mathrm{Re_{TP}}^{-n} \qquad (4)$$

with

$$\mathrm{Re_{TP}} = \frac{GD_h}{\mu_{\mathrm{TP}}} \qquad (5)$$

in which μ_{TP} is a two phase viscosity.

For a laminar flow in a rectangular channel, $n = 1$ and N is a function of aspect ratio, AR [7]:

$$N = 24(1 - 1.3553AR + 1.9467AR^2 - 1.7012AR^3 + 0.9564AR^4 - 0.2537AR^5) \qquad (6)$$

Numerous two phase viscosity models have been proposed. The models used in this study are listed in Table I. The results obtained using these models are illustrated against fuel cell working current and compared with Buie et al.'s [6] experimental data in Figure 1.

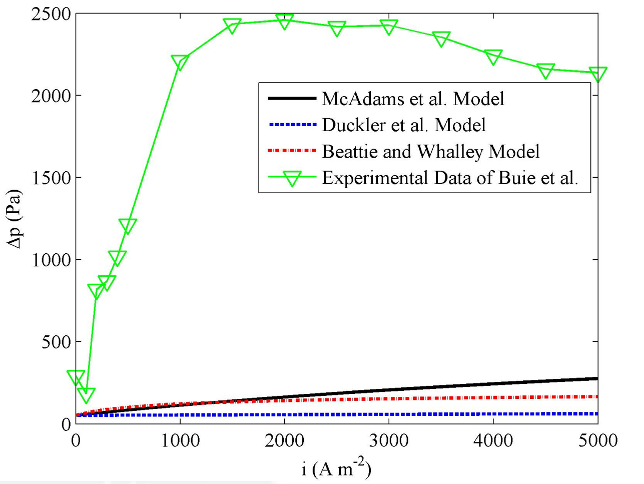

Fig. 1: Homogeneous flow models' predicted pressure drop along the anode microchannel versus current density for 1M methanol solution flowing at 200μlpm

TABLE II: Separated flow models used in this study

Model	Formula
Lockhart et al. [11]	$C = 5$
Zhang et al. [12]	$C = 21\left(1 - e^{-358/N_{\mathrm{conf}}}\right)$
Choi et al. [13]	$C = C_M(0.0012G + 1.473)$

Separated Flow Models

Separated flow models are based on a two-phase multiplier (ϕ), which is defined as:

$$\phi_L^2 = \left[\left(\frac{\Delta p}{\Delta x}\right)_{\mathrm{TP}} \bigg/ \left(\frac{\Delta p}{\Delta x}\right)_l\right] \qquad (7)$$

Lockhart and Martinelli [11] suggested that ϕ_L^2 is a function of a Martinelli parameter:

$$\phi_L^2 = 1 + \frac{C}{X_{vv}} + \frac{1}{X_{vv}^2} \qquad (8)$$

where X_{vv} is a parameter of a laminar liquid - laminar gas flow:

$$X_{vv} = \left[\left(\frac{\Delta p}{\Delta x}\right)_l \bigg/ \left(\frac{\Delta p}{\Delta x}\right)_g\right]^{0.5} = \left(\frac{1-x}{x}\right)^{0.5}\left(\frac{\rho_g}{\rho_l}\right)^{0.5}\left(\frac{\mu_l}{\mu_g}\right)^{0.5} \qquad (9)$$

In the right-hand side of Equation (6), 1 represents liquid-only pressure drop, C/X_{vv} represents mixed pressure drop, and $1/X_{vv}^2$ represents gas phase–only pressure drop. Therefore, C represents the interactional effect of the two-phase flow.

Previously proposed correlations for frictional pressure drop in a microchannel have been developed by modifying the C-value. In this study, several correlations, listed in Table II, have been used and their results are compared with experimental data in Figure 2.

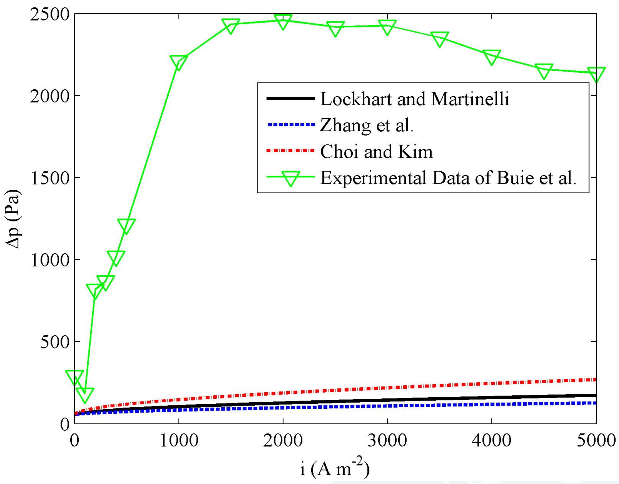

Fig. 2: Separated flow models' predicted pressure drop along the anode microchannel versus current density for 1M methanol solution flowing at 200μlpm

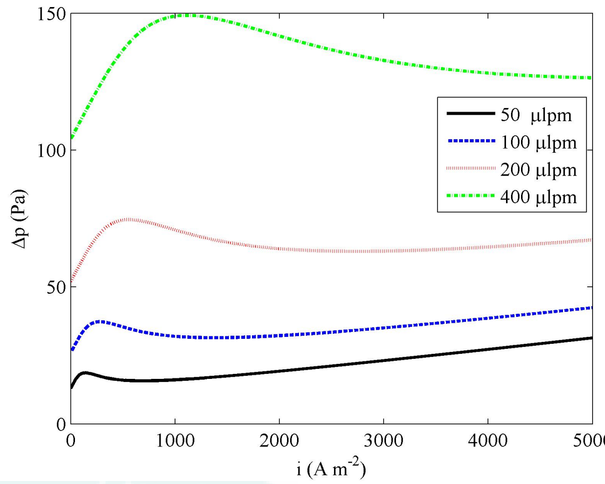

Fig. 3: Elongated bubble/slug flow model's predicted pressure drop along the anode microchannel versus current density for 1M methanol solution

Elongated Bubble/Slug Flow Model

This model is based on the works of Garimella et al. [14] and as its name suggests, consists of two regions: an elongated CO_2 bubble enclosed by a film of liquid and a section of liquid phase fuel located between these bubbles. In this study, because of the effects of interfacial components and low Reynolds number, Bretherton's [15] suggestion for the relation between bubble and slug speed is used:

$$u_{\mathrm{bubble}} \approx \left(1 + 1.29(3\mathrm{Ca})^{\frac{2}{3}}\right) u_{\mathrm{slug}} \tag{10}$$

where u_{bubble} and u_{slug} are bubble and slug average velocity and Ca is Capillary number.

To complete the model, it is assumed that the bubble length ratio is approximately equal to the void fraction of the flow. The pressure drop estimated using this model is shown in Figure 3 for different flow rates. It can be seen that model's prediction is still an order of magnitude smaller than the actual results, but it follows the real trend quite better than the previous models and thus this model is used later to modify Buie et al.'s [6] empirical model.

Proposed Semi Empirical Model

This model is a modified version of an empirical model developed by Buie et al [6] based on their experimental data, but unlike their method, considers frictional pressure drop component as well as interfacial one. In their model, void fraction is derived from experimental data, next, number of gas bubbles is approximated as a function of void fraction and at last a dimensionless pressure group which takes into account contributions of surface tension and number of slugs is correlated versus void fraction.

In this proposed model it is assumed that the total two phase pressure drop consists of frictional and interfacial components:

$$\left(\frac{dp}{dx}\right)_{\mathrm{TP}} = \left(\frac{dp}{dx}\right)_{\mathrm{fric}} + \left(\frac{dp}{dx}\right)_{\mathrm{int}} \tag{11}$$

The elongated bubble/slug flow model is used to find the frictional pressure drop. Then, in order to find a correlation for interfacial pressure drop, the experimental pressure drop data of Buie et al. [6] is modified by subtracting the amount of pressure drop that is assumed to be a result of friction from the total pressure drop:

$$\left(\frac{dp}{dx}\right)_{\mathrm{m}} = \left(\frac{dp}{dx}\right)_{\mathrm{exp}} - \left(\frac{dp}{dx}\right)_{\mathrm{fric}} \tag{12}$$

This modified pressure is processed in a similar method to the one used by Buie et al. [6] and an expression for interfacial pressure drop is obtained through forming a non–dimensional pressure group—by using number of gas bubbles, N_b, surface tension, σ, and diameter of the largest sphere inscribed in the channel, a— and then correlating it with void fraction, α:

$$\frac{\Delta p_{\mathrm{m}}\ a}{N_{\mathrm{b}}\sigma} = (1-\alpha)\left(101.9e^{-7.674\alpha} - 91.05e^{-1.831\alpha}\right) + \alpha\left(3.222\times 10^{-12}e^{28.35\alpha} + 480.4e^{-5.061\alpha}\right) \tag{13}$$

As the next step, a correlation for void fraction is sought. Inspired by previously proposed correlations for void fraction [16-18] and considering experimental data of Buie et al. [6], this expression is found as a function of volumetric quality (β):

$$\alpha = \frac{3.696\beta^{5.537}}{1 + 2.805\beta^{5.537}} \tag{14}$$

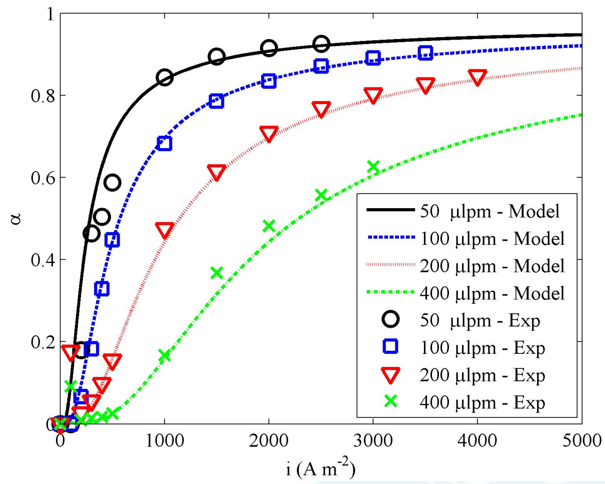

Fig. 4: Void fraction predictions of the proposed correlation compared with experimental data for 1M methanol solution

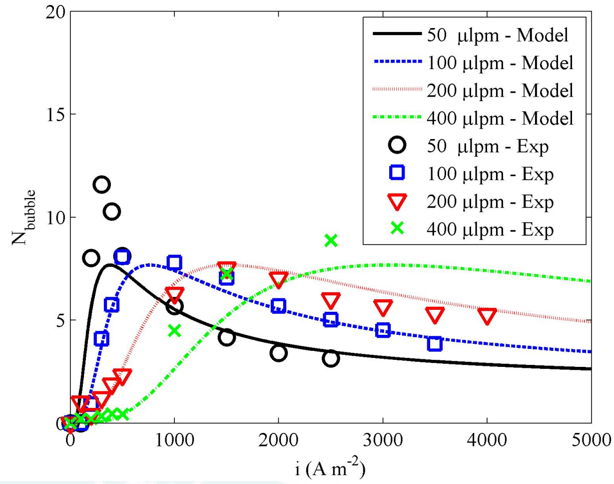

Fig. 5: The proposed correlation's predicted number of gas bubbles compared with experimental data for 1M methanol solution

with

$$\beta = \frac{Q_g}{Q} = \frac{Q_{CO_2}}{Q_{in} + Q_{CO_2} - Q_{cons}} \qquad (15)$$

in which Q_{CO_2} is the volumetric flow rate of produced CO_2 gas, Q_{in} is the inlet volumetric flow rate of the fuel solution and Q_{cons} is the volumetric flow rate of the fuel consumed through oxidation reaction in fuel cell.

The results of this correlation versus current density and for different flow rates is displayed in Figure 4 and can be seen to a be in good agreement with experimental data of Buie et al. [6].

The number of gas bubbles is estimated in a similar fashion to the original method and the expression is found to be:

$$N_b = -25.29\alpha^3 + 10.33\alpha^2 + 15.69\alpha \qquad (16)$$

Predicted number of bubbles for different flow rates using this expression is ploted against current density and compared with the expermiental data of Buie et al. [6] in Figure 5.

Results and discussions

Figure 6 shows the present model's predicted total pressure drop and compares it with Buie et al.s [6] original model and experimental data for two different flow rates. It can be seen that the present model follows the actual pressure drop trend closely and the initial rise of the pressure drop in lower current densities and the timing of this phenomenon is better captured in this model than Buie et al.'s [6]. However, the model fails to demonstrate the slight increase in the maximum pressure drop with increasing the inlet flow rate. This can be contributed to inertial effetcs which are neglected in this study.

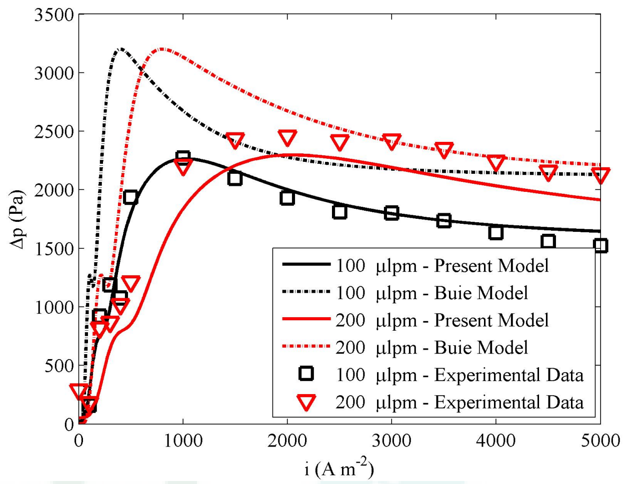

Fig. 6: Predicted total pressure drop compared with the original model and experimental data of Buie et al. [6]

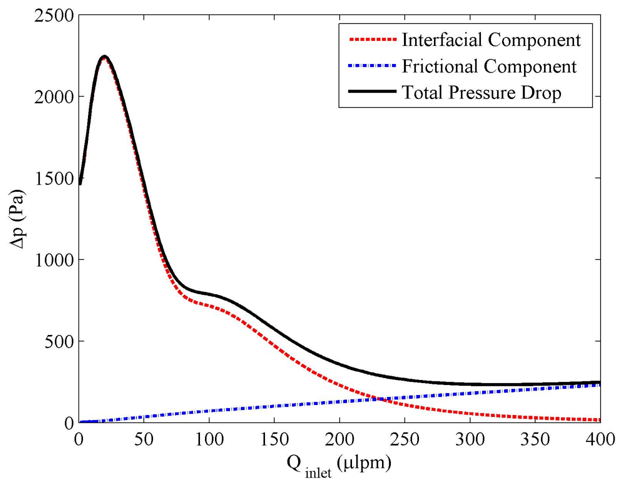

Fig. 7: Behavior of pressure drop components with increasing inlet methanol solution flow rate

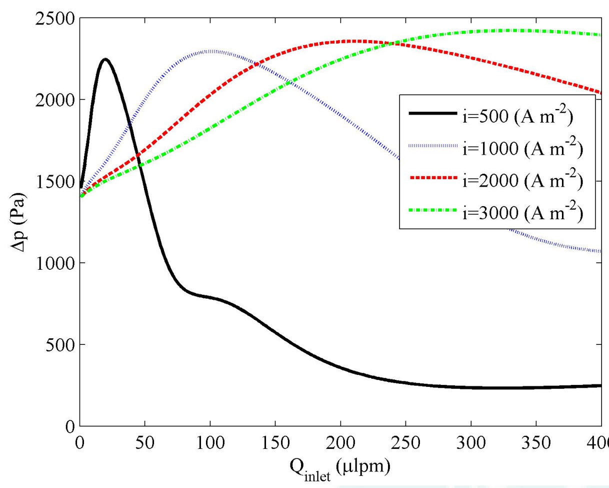

Fig. 8: Predicted total pressure drop for different working current densities against inlet methanol solution flow rate

The different responses of the two pressure drop components to increasing the flow rate of inlet methanol solution with constant working current density is illustrated in Figure 7. As expected, the frictional pressure drop increases monotonically with the flow rate, but the interfacial component's reaction needs more explanation. In a constant working current density, at very low inlet flow rates the volumetric flow rate of liquid is very small compared to gas and the flow is almost of a gas–phase–only nature. As the inlet flow rate increases the flow moves toward a two phase nature and therfore the resulting interfacial pressure drop rises. With increasing the inlet flow rate furthermore, the flow approaches a single phase liquid flow, and therefore the interfacial pressure drop decreases. It is also important to note that at low flow rates the pressure drop is dominated by interfacial effects, but as the flow rate rises this component loses its significance and frictional component increases. As a result, at relatively high flow rates the frcitional pressure drop becomes the governing component.

The behavior of the total pressure drop with increasing the inlet flow rates for different current densities is shown in Figure 8. As the current density increases, the flow reaches the two phase nature at higher flow rates and therefore the flow rate associated with maximum pressure drop increases.

Conclusion

With the purpose of improving the performance of a μDMFC system by addition of a fuel pump and recognizing hydraulic resistance as the main link between the two parts of the system, pressure drop of the fuel in the channel has been investigated. Several two phase flow models are shown to be incapable of estimating the pressure drop and so, a previously suggested empirical method is modified to predict the pressure drop in the anode of μDMFC.

The results of the new semi-empirical model suggest that using volumetric quality to estimate the void fraction and considering the viscous component of total pressure drop lead to a better prediction of the pressure drop behavior. These changes contribute to the model capturing the maximum pressure drop and difference in rise time associated with different inlet flow rates more closely.

Future works can combine theoretical, experimental and numerical methods to investigate the effect of number of gas bubbles and inertial forces as well as interfacial and viscous forces on pressure drop in μDMFC anode's microchannel more comprehensively.

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