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Conjugate mass transfer in gas channels and diffusion layers of fuel cells

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Conjugate Mass Transfer in Gas Channels and Diffusion Layers of Fuel Cells

S. B. Beale

Mem. ASME
National Research Council,
Montreal Road,
Ottawa, Ontario K1A 0R6 Canada
e-mail: steven.beale@nrc-cnrc.gc.ca

Prediction of mass transfer effects is a key element in fuel cell design. In this paper, the results of a generalized analysis appropriate to a wide range of designs and flow conditions are presented. Mass transfer in a rectangular gas passage, diffusion layer, and the combination of the two is considered. Fully developed viscous flow is presumed to occur within the passage, while the incompressible form of Darcy's law is prescribed for the diffusion layer. The mathematical foundations for a simple mass transfer analysis are presented. Detailed calculations are then performed by means of a computational fluid dynamics code. These results are then correlated according to the analytical methodology in terms of nondimensional numbers appropriate to mass transfer analysis; namely, the overall mass transfer driving force as a function of the blowing parameter. Parametric studies are performed for a range of geometries, as characterized by the aspect ratio and blockage factor. It is shown that a simple solution for the overall driving force may readily be obtained from the two individual solutions for the conjugate mass transfer problem. This solution is quite general in its nature, and may readily be used to predict concentration polarization effects for a variety of fuel cells. [DOI: 10.1115/1.2393300]

1 Introduction

Fuel cells have become the subject of much active engineering research in recent times. For fuel cells to be adopted by the public, it is required to minimize electrical losses in order to increase the overall efficiency. Losses may be due to charge transfer (activation/kinetic) factors, electrical resistance of ionic and electronic conductors, or mass transfer losses, which are also referred to as concentration polarizations or concentration overpotentials. The latter matter is the subject of this paper.

Computer models have been used effectively in the design and analysis of fuel cells. These range from simple algorithms to detailed codes. For a recent review of the application of computational fluid dynamics (CFD) to fuel cells (see Ma et al. [1]). Because of the complexity of the physical structure and the transport phenomena inherent in fuel cells, large scale calculation procedures are very time consuming. There is much benefit to employing simplified problem formulations; Beale and Zhubrin [2] compared detailed and simplified CFD methodologies, using a distributed resistance analogy, for an idealized fuel cell stack where the channels were in the form of planar ducts, and the diffusion layers were entirely absent. The goal of the present work is to demonstrate that a simplified mass transfer formulation may be extended in application to the design and development of more realistic fuel cell designs.

The majority of present-day CFD and other mathematical models of fuel cells assume Fick's law to be applicable, for the rate of mass transfer due to diffusion

$$j'' = \Gamma \text{ grad } m \quad (1)$$

where $\Gamma = \rho D$ is referred to as an exchange coefficient. For many situations, this is quite a reasonable assumption. (The reader will note that in this text, the convention first proposed by Jacob [3], whereby a "dash" represents per unit length and a "dot" represents per unit time, is adopted.) In order to develop simple models, it is necessary to make an additional commonly adopted engineering assumption, and to postulate that the magnitude of the diffusion

flux is proportional to the difference between the wall and bulk mass fractions

$$j'' = g(m_w - m_b) \quad (2)$$

where m_w is the boundary or wall value, m_b is the bulk value of mass fraction, and g is a conductance or mass transfer coefficient.

Previous work by the present writer focused on mass transfer in the gas passages of the fuel and oxidant [4]. In the present work, the analysis is expanded to consider combined mass transfer in both the gas channels and the diffusion layers, typically found in most common fuel cell types. Mass transfer is a highly interdisciplinary activity and a variety of methodologies have been adopted in the field of fuel cell technology. The goal is to put the analysis on a rational basis, consistent with standard engineering techniques.

Figure 1 is a schematic of the problem under consideration. Gas flows along a rectangular channel, $W_1 \times H_1$, in the streamwise or axial direction, with the local bulk mass fraction of the transferred species being denoted by m_b . The transferred substance passes through a gas diffusion layer in a direction perpendicular to the electrode surface, where it is produced or destroyed at some rate $\dot{m}_2''$, corresponding to current density i'' . Let m_1 and m_2 refer to the average mass fraction of the transferred substance on either side of the gas diffusion layer. Let it be supposed that

$$\dot{m}_1'' m_1 = \dot{m}_1'' m_1 + g_1(m_1 - m_b) \quad (3)$$

$$\dot{m}_2'' m_2 = \dot{m}_2'' m_2 + g_2(m_2 - m_1) \quad (4)$$

where m_i is the value of m at the transferred substance state. For mass transfer in the absence of chemical reactions, the transferred substance state may be considered as a state sufficiently far from the interface, such that only convection (and not diffusion) is significant and $0 \leq m_i \leq 1$. Therefore, for a single (pure) transferred substance, $m_i = 1$.

However, when chemical reactions occur m_i can assume any value, $-\infty \leq m_i \leq \infty$. This then is computed according to [5–8]

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Fig. 1 Schematic of gas channel and diffusion layer

$$m_i = \frac{\dot{m}_i''}{\dot{m}''} \quad (5)$$

where $\dot{m}'' = \sum \dot{m}_i''$, and $\dot{m}_i''$ are the mass fluxes of the individual chemical species.

The channel and diffusion layer aspect ratios α_1 , and α_2 , and the blockage factor β are defined as

$$\alpha_1 = \frac{H_1}{W_1} \quad (6)$$

$$\alpha_2 = \frac{H_2}{W_2} \quad (7)$$

$$\beta = \frac{W_1}{W_2} \quad (8)$$

where $0 \leq \beta \leq 1$. The parameters α_1 , α_2 , and β will vary for different fuel cell designs. The case $\beta = 1/2$ corresponds to the situation where the gas channels and the solid interconnect ribs for a solid oxide fuel cell (SOFC) or lands of the bipolar plates for a proton exchange membrane fuel cell (PEMFC) are of equal widths. This situation is frequently encountered in practice. A value of $\alpha_2 = 1/8$ is also typical for the diffusion layers in many modern-day PEMFCs.

The analysis can proceed in two possible directions: (a) Detailed numerical calculations may be performed using CFD and (b) a fundamental mathematical analysis, based on mass transfer theory, may be used. A combination of these approaches is developed further, below.

In the present paper, calculations were performed for fluid flow and mass transfer in (a) rectangular ducts, (b) partially blocked porous media, and (c) the combined problem. Only single-phase flow is considered in the present work. Fully developed flow and mass transfer are presumed. The present author has encountered channel Reynolds numbers ranging from $0 \leq Re \leq 200$, in real fuel cell applications; i.e., well within the laminar regime. Some details of the method by which the boundary conditions were prescribed are given in [9]. The scope of the work is restricted to isothermal single-phase mass transfer with constant properties.

Fig. 2 Schematic of gas channel

The finite-volume CFD code PHOENICS [10] was used to perform the calculations.

2 Channel Flow

Figure 2 illustrates the problem of flow in a channel of dimensions $W_1 \times H_1$. Fluid containing a mixture of species enters and exits the duct in the axial direction. A fraction of the transferred species is removed across the upper surface $c-d$. The other three surfaces are impervious to mass transfer. Equation (3) may be re-written in terms of a mass transfer driving force B_1

$$B_1 = \frac{m_b - m_1}{m_1 - m_i} \quad (9)$$

such that the mass flux $\dot{m}_1''$ across $c-d$ is given by [5]

$$\dot{m}_1'' = g_1 B_1 \quad (10)$$

Equation (10) is of fundamental importance since it states that the mass flux $\dot{m}_1''$ is proportional to the driving force B_1 ; the constant of proportionality being the conductance, or mass transfer coefficient g_1 . It has thus been referred to in the past as the "Ohm's law" of mass transfer. Note, however, that the conductance g_1 is not constant, but varies as a function of $\dot{m}_1''$.

For convenience, a blowing parameter b_1 or nondimensional mass flux is defined as

$$b_1 = \frac{\dot{m}_1''}{g_1} \quad (11)$$

where g_1^* is the value of g_1 in the limit $\dot{m}_1'' \rightarrow 0$. The blowing parameter is essentially a Peclet number; i.e., the ratio of convection to diffusion. Thus, for small b , diffusion is the dominant mechanism for mass transfer, and conversely for high b , convection predominates. This definition obviates the need to define a length scale, such as a hydraulic diameter D_h , associated with the more conventional definition of the wall Peclet number [11]: $Pe = 4D_h \dot{m}_1'' / \Gamma$.

For the case of mass transfer in rectangular ducts, the wall mass fraction m_1 is not constant and therefore B_1 is computed from a mean value

$$m_1 = \frac{1}{A} \int m dA \quad (12)$$

where the integration is conducted over the surface area of the wall ($c-d$ in Fig. 2). Thus, m_1 and g_1 are to be considered as arithmetic and harmonic mean values, respectively, m_i is known, and m_b varies only in the streamwise (axial) sense.

Figure 3 is a comparison of the numerical results obtained by the present writer, with those of Schmidt as presented in the book by Shah and London [12] in terms of the zero-flux Sherwood number Sh_1^* , defined as

Fig. 3 Values of Sh_1^* for rectangular ducts as obtained here, compared with data of Schmidt, from Shah and London [12]

$$Sh_1^* = \frac{g_1^* D_h}{\Gamma} \quad (13)$$

to be considered a function of the duct aspect ratio α_1 . Since if there is no mass flux, the driving force (and concentration gradient) must therefore be zero; values of Sh_1^* were obtained by solving for an additional scalar for which convection was de-activated. An alternative is to simultaneously set $\dot{m}''$ to a very small number and m_i to a very large number. (Values of Sh_1 based on the latter consistently approached the former as $b_1 \rightarrow 0$.)

Numerical calculations for flow in planar and square ducts were previously presented in [9]. Figure 4 shows results for numerical calculations performed for rectangular ducts with aspect ratio $\alpha_1 = \frac{1}{5}, \frac{1}{2}, 1, 2, 5$. These have been plotted in terms of the driving force as a function of blowing parameter on a logarithmic scale, $\ln(1+B_1)$ versus b_1 , in order to remove bias. It can be seen that the data are reasonably linear over the range $-1 \leq b_1 \leq 1$, which suggests that the solution to the 1-D convection-diffusion equation

$$B_1 = \exp(b_1) - 1 \quad (14)$$

may be used to predict B_1 given g_1^* , and $\dot{m}''$ for fully developed mass transfer in rectangular ducts. Outside of this range, it can be seen that the quantity $\ln(1+B_1)$ is higher than predicted by simple 1-D theory, regardless of whether $b_1 \ll -1$ or $b_1 \gg +1$. For very high mass transfer rates, therefore, a quadratic form

Fig. 4 Mass transfer driving force B_1 as a function of blowing parameter b_1 for gas channel

$$\ln(1+B_1) = a_1 b_1 + a_2 b_1^2 \quad (15)$$

is more appropriate. Values of this regression curve with $a_1 = 0.9647$ and $a_2 = 0.0868$ are illustrated in the figure. Even though the characteristic is not entirely linear, all the data still fall onto a single characteristic curve over the range $1/5 \leq \alpha_1 \leq 5$ and $-3 \leq b_1 \leq 3$. Increasing the gas channel aspect ratio α_1 causes the conductance g_1^* (and hence g_1) to decrease, as shown in Fig. 3. However, the aspect ratio does not impact on mass transfer, as correlated in the nondimensional form (Fig. 4), where essentially a "universal" distribution is obtained. For $-1 \leq b_1 \leq 1$ the "linear" form $\ln(1+B_1) = b_1$ is perfectly adequate. Although in principle it is possible to obtain arbitrarily large values of $|b_1|$, by increasing the main flow Reynolds number, the same practice cannot be adopted for the diffusion layer and the situation $-1 \leq b_1 \leq 1$ will likely be encountered in a large majority of cases.

3 Diffusion Layer

For fluid flow in the gas diffusion layer, the incompressible form of Darcy's law is presumed to apply

$$U = -\frac{k}{\mu} \text{grad } p \quad (16)$$

where $U = eu$ is the superficial or filter velocity, u is the interstitial or pore velocity, k is the permeability, and μ is the dynamic viscosity. This is easily coded into a CFD code by the introduction of a linearized source term in the momentum equations. The overall pressure drop between the inlet and exit must be nominally the same for both the gas channel and the diffusion layer, assuming uniform pressure in the inlet and outlet manifolds. It is therefore a reasonable assumption that the axial component of velocity in the diffusion layer is taken as negligibly small, since otherwise large differences in the axial pressure gradient in the diffusion layer and the channel would arise. Moreover, it is assumed for the purpose of the present analysis that axial diffusion is also negligible. These assumptions are relaxed below. Thus, the present problem reduces to a two-dimensional (2-D) situation, greatly simplifying the analysis.

For mass transfer an effective diffusion coefficient is sometimes defined according to $\gamma_{\text{eff}} = \Gamma / \tau^2$, where τ is tortuosity [13]. This allows for terms associated with redistribution of m , in the diffusion layer to be accounted for in terms of an interstitial diffusion flux: $j'' = -\gamma_{\text{eff}} \text{grad } m$. The associated superficial diffusion flux is just $J'' = \epsilon j''$, so the effective exchange coefficient is $\Gamma_{\text{eff}} = \epsilon \gamma_{\text{eff}}$, and hence the equation for steady mass transfer in diffusion layer is of the usual form

$$\text{div}(\rho U m) = \text{div } \Gamma_{\text{eff}} \text{grad } m \quad (17)$$

The quantity ϵ / τ^2 may simply be replaced by the exchange coefficient ratio $\Gamma_{\text{eff}} / \Gamma$, which is employed in the remainder of this paper.

3.1 Boundary Conditions. The choice of boundary conditions must be made carefully, as these will affect the final flow-field results. These were selected as follows. (i) The external pressure p_∞ across $c-d$ in Fig. 5, was presumed constant and the continuity (pressure-correction) boundary condition coded as a linear source term in terms of the local pressure

$$\dot{m} = A \frac{\rho k}{\mu \delta y} (p_\infty - p_p) \quad (18)$$

where ν is kinematic viscosity, A is cell area, and δy cell center-to-wall distance. This has the effect of setting the pressure p_p in the computational cells within the diffusion layer that are immediately adjacent to channel such that the difference between p_p and $p_\infty = 0$, is consistent with Darcy's law (Eq. (16)). (ii) For the upper boundary the normal velocity at the wall, and hence the mass flux $\dot{m}''$, was presumed constant along $f-g$. This represents

Fig. 5 Schematic of diffusion layer

the ideal case corresponding to uniform current density at the electrode wall. The mass flux and hence the nondimensional blowing parameter were varied as the independent variable. (These are related to the mean current density for any given fuel cell according to Faraday's law.) No constraint was imposed on the tangential velocity. This combination of pressure and mass-flow boundary conditions were always the same, regardless of whether the latter were prescribed as inflow (blowing) or outflow (suction) along $f-g$. For mass transfer, it is assumed that there is mass transfer between the wall and a reservoir at transferred substance state m_p , as shown in Fig. 5. Thus the total (convective plus diffusive) flux is prescribed as $m_2''(m_i - m_p)$ where m_p is the in-cell value. This was prescribed as a linearized term for injection and as a fixed source for suction [14]. At the channel boundary ($c-d$, Fig. 5), the convective and diffusive fluxes were prescribed separately, the former as $m_1''(m_p - m_p)$, where m_p is the previous value of m_p and the latter as $g_1(m_b - m_p)$. Values of g_1 were estimated using 1-D theory as

$$g_1 = g_1^* b_1 / (\exp b_1 - 1) \quad (19)$$

where g_1^* is obtained from Eq. (13).

3.2 Numerical Data. Numerical solutions to Eqs. (16) and (17) were obtained using the finite volume method. The results of these calculations are shown in Figs. 6–9. Figure 6 shows pressure contours and velocity vectors for the case $\alpha_2 = 1/8$, $\beta = 1/2$. Because of the symmetry, only one-half of the domain was considered, as shown. A porous media flow is a potential flow (see Fig. 6 and Eq. (16)), so the form of the velocity and pressure fields are invariant, for any given geometry. Though the magnitude of the pressure field varies as a function of the velocity, the form is identical; regardless of the magnitude and sign of the velocity field, provided the diffusion layer is sufficiently impermeable that Darcy's law is valid. This can easily be proved by substituting the velocity from Darcy's law into the continuity equation, $\text{div } \rho U = 0$, it immediately follows that the pressure is a harmonic func-

Fig. 6 Normalized pressure and velocity fields, $\alpha_2 = 1/8$, $\beta = 1/2$, $b = -1$

Fig. 7 Normalized concentration fields, $\alpha_2 = 1/8$, $\beta = 1/2$

tion, $\text{div grad } p = 0$, for constant k, μ, ρ . It can be seen from Fig. 6, that the flow accelerates in the corner region (labeled "c" in Fig. 6), where the pressure gradient is a maximum, as a result of the well known properties of harmonic functions. Thus, an important conclusion of this study is that even if the flow within the channel is uniform; it is quite nonuniform just inside the diffusion layer. Many fuel cells are constructed with diffusion layers sufficiently impermeable that Darcy's law may be considered an appropriate empirically based mathematical description for the motion of the fluid. For some fuel cell designs, however, the gas diffusion layers may be highly porous and Darcy's law must be modified to account for boundary layer or viscous effects, for example, using Brinkman's theory; also if the Reynolds number (based on a pore diameter or the like) is sufficiently high, inertial effects may become significant. Under either of these circumstances, the flow-field and pressure distributions will deviate from the universal form of the solution to Darcy's law.

Contours of the scalar mass fraction (Fig. 7) also assume a Laplacian form for "zero" (i.e., very small) mass transfer, since $\text{div } \Gamma_{\text{eff}} \text{ grad } m = 0$. For finite mass transfer rates, however, isovalues are "pushed up" or "pulled down" depending upon the direction of U , due to the nonlinear behavior of the convection-diffusion system. The reader will note that the range of contours in Fig. 7 vary for the two cases, and become negligibly small as $b \rightarrow 0$. In the limit $b = 0$ there is no driving force (concentration gradient), as there is no mass transfer. (For some catalytic reactors, mass transfer can occur as $b \rightarrow 0$, because $m_i \rightarrow \pm\infty$, however that situation does not normally arise for fuel cells.) As the aspect ratio $\alpha_2 \rightarrow 0$, concentration variations become large. Variations in pressure and concentration are a matter for concern in fuel cell design as they may lead to changes in the local electric field potential and current density. These will occur at moderate mass flow rates, even if the mass flow rate (current density) is entirely uniform.

For the 1-D case corresponding to zero blockage ($\beta = 1$), it is readily apparent that $g_2^* = \Gamma_{\text{eff}}/H_2$. For the general case, it is convenient to define a pseudo-Sherwood number (essentially a non-dimensional conduction shape factor) in terms of the diffusion layer height, according to

$$\text{Sh}_2^* = \frac{g_2^* \Gamma_{\text{eff}}}{H_2} \quad (20)$$

Figure 8 shows computed values of the shape factor Sh_2^* obtained from numerical solutions of the conduction equation. It can be seen that Sh_2^* decreases from $\text{Sh}_2^* = 1$ when $\alpha = \beta = 1$, as either α or β decrease. These values were obtained assuming a constant transformed substance-state at the top boundary, but with a linearized source term $g_1(m_b - m_w)$, with constant g_1 , as previously discussed (Eq. (19)). Values of Sh_2^* obtained assuming a constant transformed substance state at both top and bottom walls differ from these values by around 5%. This is due to the fact that local values of both g_1 and m_1'' vary (see Fig. 6); either way, an engi-

Fig. 8 Sh_2^* as a function of blockage factor

neering approximation must be made.

Figure 9 shows values of the mass transfer driving force as a function of the blowing parameter, for mass transfer in the diffusion layer. The mass transfer driving force in the diffusion layer is defined as

$$B_2 = \frac{m_1 - m_2}{m_2 - m_t} \quad (21)$$

It can be seen that for $\alpha_2 = \frac{1}{2}$, the results correlate extremely well with the 1-D solution, but as α decreases there are departures as $|b_2| > 1$. For these cases, a cubic polynomial

$$\ln(1 + B_2) = a_1 b_2 + a_2 b_2^2 + a_3 b_2^3 \quad (22)$$

has been used to correlate to B_2 . Values given in Table 1 were obtained as a regression fit to the data in Fig. 9. Values of the shape factor or "Sherwood number" for the case $\beta = \frac{1}{2}$ are also provided.

Fig. 9 B_2 vs b_2 . Diffusion layer $\beta = \frac{1}{2}$.

Table 1 Coefficients for data used in Fig. 9, $\beta = \frac{1}{2}$

α_2	Sh_2^*	a_1	a_2	a_3
1	0.8879	1	0	0
1/2	0.7986	0.9480	-0.0205	-0.0055
1/4	0.6500	0.9325	0.0154	-0.0070
1/8	0.4113	0.8493	-0.0129	-0.0143
1/16	0.1794	0.6350	-0.2560	-0.0103

Fig. 10 Computational grid

4 Conjugate Mass Transfer

4.1 Theory. Equations (3) and (4) satisfy the identity

$$\dot{m}_2'' = \beta g_1 B_1 = g_2 B_2 \quad (23)$$

One may conveniently write

$$\dot{m}_2'' = gB \quad (24)$$

where the overall driving force B is defined as

$$B = \frac{m_b - m_2}{m_2 - m_t} \quad (25)$$

Let the overall blowing parameter b be defined according to

$$b = \frac{\dot{m}_2''}{g} \quad (26)$$

$$g^* = \frac{\beta g_1 g_2^*}{\beta g_1 + g_2^*} \quad (27)$$

It follows that

$$b = b_1 + b_2 \quad (28)$$

Equation (28) is used to compute the overall driving force from the two individual values.

4.2 Results. Figure 10 illustrates a typical grid employed in this work, showing the channel, diffusion layer, and solid regions. In view of the symmetry a domain of $\frac{1}{2}W_2 \times (H_1 + H_2)$ was employed, as shown. Two specific cases were considered: high aspect ratio $\alpha_2 = \frac{1}{2}$, and low aspect ratio $\alpha_2 = \frac{1}{8}$, the latter corresponding to a typical present-day PEMFC. For the latter case the ratio $\Gamma_{\text{eff}}/\Gamma$ was also varied from a maximum $\Gamma_{\text{eff}}/\Gamma = 1$, to the case considered in the Appendix, with $\Gamma_{\text{eff}}/\Gamma = 0.3536$. In all cases, it was assumed that $\alpha_1 = 1$ and $\beta_2 = \frac{1}{2}$, corresponding to a square gas channel, with land (solid region) and channel being of equal width.

Figure 11 shows typical flow-field results in terms of velocity vectors and pressure contours. Figure 12 illustrates concentration profiles in the combined assembly for values of $\Gamma_{\text{eff}}/\Gamma = 1$, and $\Gamma_{\text{eff}}/\Gamma = 0.3536$. Figures 13 and 14 show mass transfer driving forces B_1 , B_2 , and B as defined in Eqs. (9), (21), and (25), as function of blowing parameters b_1 , b_2 , and b in the range $-2 \leq b_2 \leq 2$.

Fig. 11 Pressure contours and velocity vectors

5 Discussion

It can be seen from Fig. 11 that axial velocities in the channel are large in comparison to those in the diffusion layer. Conversely axial pressure losses in the channel, are negligibly small compared to cross-wise gradients in the diffusion layer. Comparison of the results of Fig. 6 and Fig. 11 reveal the pressure and velocity fields to be essentially identical for the diffusion layer (only) and conjugate channel-diffusion layer problems. The concentration profiles shown in Fig. 12 are also inherently similar to the results of Fig. 7. It can be seen from Fig. 12 that there are larger mass fraction gradients in the diffusion layer, as the exchange coefficient ratio Γ_{eff}/Γ increases, for a given value of the blowing parameter b_2 . In general the diffusion layer is going to be the rate-limiting factor since in the channel one can increase the through-plane Reynolds number and ensure the wall value is such that $0 \leq m_1 \leq 1$. The same situation is not possible in the diffusion layer: due to the impermeability of the porous media, the through-plane velocity is negligibly small; i.e., the motion is inherently 2-D.

The pressure gradient across the diffusion layer is generally much larger than the lateral gradient in the channel, and closely resembles that shown in Fig. 6. Concentration gradients, however, occur across both the channel and the diffusion layer. The relative magnitude of these depend on the ratio Γ_{eff}/Γ and also geometry. Thus, as Γ_{eff}/Γ decreases, the concentration gradients in the diffusion layer increase. Values of Γ_{eff}/Γ may be expected to range from 1 down to $\frac{1}{5}$ depending on the material used in the fuel cell membrane/electrolyte. See Litster and Djilali [15] for a discussion of the range of Γ_{eff} in PEMFCs.

It is desirable to maintain $\Gamma_{eff}/\Gamma \ll 1$, since if $m_1 \rightarrow m_b$, it is possible to maximize the limiting current density, i''_{lim} and associated blowing parameter, and limiting driving force

Fig. 12 Normalized concentration contours, $b_2 = -1$

$$B_{lim} = \frac{m_b}{m_i} \quad (29)$$

Trial calculations of B_{lim} and i''_{lim} are to be found in the Appendix.

Figures 13 to 15 show values of B_1 , B_2 , and B as a function of b_1 , b_2 , and b for the conjugate mass transfer problem. Figure 13 is for a very thick diffusion layer with $\alpha_2 = \frac{1}{2}$, and $\Gamma_{eff}/\Gamma = 1$, Figure 14 is for a thin diffusion layer, $\alpha_2 = \frac{1}{8}$ with $\Gamma_{eff}/\Gamma = 1$, and Figure 15 shows the case $\alpha_2 = \frac{1}{8}$ again but with $\Gamma_{eff}/\Gamma = 0.3635$, corresponding to the Appendix.

For the results of Fig. 13, values of B_1 , B_2 , and B all approximate the 1-D solution over a wide range of the blowing parameter. The driving forces in the channel are sufficiently small that variations are relatively minor. Under these circumstances high mass flows (current densities) can be achieved without reaching the

Fig. 13 B versus b . Conjugate problem, thick diffusion layer, $\Gamma_{eff}/\Gamma = 1$.

Fig. 14 B versus b . Conjugate problem, thin diffusion layer, $\Gamma_{\text{eff}}/\Gamma = 1$.

mass transfer limit, due to the concentration gradient being relatively small in the transverse direction. At very high mass flow rates, the profile becomes nonlinear; however, in most fuel cells, B_{lim} and i''_{lim} will have been reached before this.

The results of Fig. 15 are consistent with those of Fig. 14. Because the exchange coefficient ratio is smaller, values of the channel blowing parameter b_1 are correspondingly smaller than those in the diffusion layer. The straight lines in Fig. 13 and 15 are the regression lines based on the assumption $B = \exp(b) - 1$. It can be seen that this simple analysis yields quite realistic results, and only for $b > 1$ are appreciable errors encountered. Trial calculations (see the Appendix), suggest that for present-day fuel cells, $b < 1$, and therefore a 1-D analysis based on values of Sh_1^* and Sh_2^* is generally adequate.

Comparison of the results of Figs. 13 and 14, suggest that for $\alpha_2 = \frac{1}{8}$, i.e., a thin diffusion layer, higher values of b and hence B for a given value of $\dot{m}''$ (ie for a given current density) will arise. This is due to values of the shape factor Sh_2^* decreasing as α_2 decreases (Table 1). Moreover if α_2 is reduced by decreasing the height H_2 for a given width, this implies $g_2^* = \text{Sh}_2^* H_2 / \Gamma_{\text{eff}}$ will be further reduced according to Eq. (20). This results in the mass transfer limit being reached sooner for low aspect ratio than for high aspect ratio diffusion layer geometry. Inspection of Figs. 6 and 7 reveal that this is to be anticipated; by virtue of the elongated shape of the diffusion layer; isovalues of mass fraction are inevitably oriented along rather than across the diffusion layer resulting in significant changes in mass fraction in the x -direction. The implication is that a thin diffusion layer is less effective from

Fig. 15 B versus b . Conjugate problem, thin diffusion layer, $\Gamma_{\text{eff}}/\Gamma = 0.3635$.

the perspective of mass transfer. Also shown in Figs. 13 and 14 are the polynomials used to approximate the channel and diffusion layer driving forces. It can be seen that the channel characteristic closely follows the quadratic regression curve, and that the diffusion layer characteristic clearly approximates the cubic polynomial, except for $b < -1$, where some departures are observed.

It is to be noted that the conjugate mass transfer problem differs from the two individual problems in that a constraint at surface 1 (gas channel/diffusion layer) boundary has been removed, and hence some deviation in the mass fraction distribution from the two separate problems is to be expected. This, together with the fact that smaller values of b_1 result in a higher overall blowing parameter b and driving force B for the conjugate problem compared to the individual diffusion layer/channel problems, may partially explain why the conjugate problem is, if anything, closer to the 1-D solution than the results for Figs. 4 and 9. Values of g_1^* and g_2^* used here to compute b were based on the individual solutions, not those computed for the conjugate problem, though there is no problem in obtaining the latter as part of the calculation procedure.

In this study, a pure slip condition was imposed at the diffusion layer-electrode (tangential velocity) boundary. While a conventional no-slip boundary condition is not considered applicable, the wall (surface 2 in Fig. 1(a)), will locally influence the flow-field either generating shear, for a solid wall, or perhaps accelerating the flow, for example, if the electrode were a porous media substantially more permeable than the diffusion layer itself.

Trial calculations suggest that one is very unlikely to ever obtain values outside the range $-1 \leq b \leq 1$, for conventional SOFCs and PEMFCs. Only for very pure substances is it possible to achieve such high rates of mass transfer, and since a fuel cell involves electrochemical reactions, it is inevitable that at either the cathode (PEMFC) or the anode (SOFC) both reactants and products are present in the mixture and therefore a limiting current will be reached. (For the PEMFC considered in the Appendix, $b_{\text{lim}} = 0.136$.)

It can be shown that the relationship among B_1 , B_2 , and B may be expressed as follows

$$B = B_1 + B_2 + B_1 B_2 \quad (30)$$

which is consistent with the substitution of Eq. (28) into Eq. (14). The reader will note that only for low mass flow rates does $B = B_1 + B_2$ and $g = \beta g_1 g_2 / (\beta g_1 + g_2)$. At high mass transfer rates, the overall driving force deviates progressively from the sum of the individual B -values, and the conductance from the harmonic mean.

The overall driving force is to be considered a function of Sh_1^* , Sh_2^* , β , $\Gamma_{\text{eff}}/\Gamma$, and b . For the case considered in the Appendix, which corresponds to the results of Fig. 14, $\beta g_1^*/g_2^* \approx 2.5$. This suggests that, even though the diffusion layer is thin, mass transfer resistance in the diffusion layer is dominant, though mass transfer in the channel is still significant.

The significance of the B versus b characteristic is that it allows wall values to be computed from those in the bulk. In electrochemical devices, the reaction rate i'' and hence the mass flux $\dot{m}''$ and blowing parameter b are generally known. The driving force $B(b)$ may be readily computed. Knowledge of the driving force allows for the mass fraction m_2 to be computed from the bulk fluid value as follows [16]

$$m_2 = \frac{m_b + B m_i}{1 + B} \quad (31)$$

Bulk mass fractions of hydrogen, oxygen, water, etc. are generally obtained from species balances based on the prescribed value of i'' . It is common in chemical engineering texts to consider concentration defined in terms of mole fraction x_i

$$x_i = \frac{m_i}{M_j} M \quad (32)$$

where

$$M = \sum_j x_j M_j = \frac{1}{\sum_j m_j / M_j} \quad (33)$$

Wall mole fractions are generally required for both the Nernst and Butler-Volmer equations (it is, of course, possible to recast these in terms of the mass fractions). These are then used to correct the cell potential and current density, iteratively, until a suitable convergence criterion is met. In electrochemistry, mass transfer losses are sometimes written explicitly, as a sum of individual concentration overpotentials, which are individually given by

$$\eta = -\frac{RT}{nF} \ln \left[\frac{x_b}{x_w} \right] \quad (34)$$

In a hydrogen fuel cell, $n=2$, 4, and 2 for hydrogen, oxygen, and water, respectively. The Appendix contains a sample calculation for concentration overpotential.

In this paper it was assumed that the rate of mass transfer $\dot{m}''$ at the electrode boundary, was constant. In a fuel cell, this implies local variations of the current density $-i''$ to be negligibly small. However, the current density is itself a function of the local mass fractions, since the change in the Nernst half-potential Φ across any given electrode may be written as

$$\Delta\Phi = \Delta\Phi^0 \pm k(\ln x^v) + \dots \quad (35)$$

and the local current density may be expressed, rather loosely, as $i'' = -\sigma \text{ grad } \Phi$ (neglecting losses).

Whether the current density is uniform at the wall will depend on how much changes in mass fraction m affect the Nernst potential; i.e., the relative magnitude of the two terms on the right side of Eq. (35). In many situations, changes in the Nernst potential (or half-potential) due to m are negligibly small and i'' is locally constant. At sufficiently high values of mass flux, the quantity $\dot{m}''$ can no longer be presumed constant at the wall, and this in turn will affect the boundary values and hence the solution to the problem. The effect of $\dot{m}''$ on the distribution of m at the wall has been illustrated. The inverse analysis is problem-specific, and cannot readily be generalized. However, it may be that the current density does not have a strong influence on the concentration field: if the diffusion layer is sufficiently impermeable the velocity field within the porous media is a function of the pressure distribution at the electrode boundary not the velocity (current density) immediately outside the region. Future studies might include prescribing a linear or other non-constant profile and studying the deviation of the B versus b characteristic.

In the present study, the diffusion layer was presumed to be sufficiently impermeable that Darcy's law could be applied. In many practical fuel cell designs both boundary-layer and inertial effects may be present [17]. Under these circumstances the Brinkman-Forchheimer form of Darcy's law may be appropriate. Moreover some materials display anisotropic permeability in different directions. Many fuel cells also contain several diffusion layers of different permeabilities. Another concern is the presence of lateral pressure gradient (e.g., across serpentine channel designs), which can cause secondary flows [18].

Future work should consider these and other factors, as well as the case in which three distinct media are present: micro-channels, passive porous diffusion layers, and an active porous electrode region of finite thickness, with an associated bulk-to-wall driving force associated with electrochemical catalytic reaction. Several studies have shown that the application of Fick's law to mass transfer in fuel cells is quite reasonable when the oxidant and fuel are both gases. For situations where, say, a multi-species liquid fuel is employed, and if there are substantial differences in the

exchange coefficients, there is no recourse other than to consider the Stefan-Maxwell equations [19], and the simple methodology developed in this paper cannot then be applied, as multiple diffusion rates are present. However, application of the Stefan-Maxwell equations in diffusion layers (where volume-averaging is standard practice) should be considered questionable. Fortunately the majority of modern day fuel cells, such as PEMFCs and SOFCs, employ gaseous working fluids, to which the present method, based upon Fick's law and the notion of the mass transfer coefficient or conductance, may readily be applied.

6 Conclusions

CFD calculations were performed for the problem of single-phase mass transfer in fuel cell microchannels, gas diffusion layers, and a combination of these. The results were correlated in terms of a mass transfer driving force B as a function of blowing parameter b . For the gas channel, the driving force approximates the form of the 1-D solution in the range $-1 \leq b \leq 1$. Outside of this range, observed values of B were typically higher than the 1-D situation. The data nominally fall on a single characteristic curve, regardless of the aspect ratio α_1 . For mass transfer in the diffusion layer, the solution is a function of both the aspect ratio α_2 and the blockage factor β . As either $\alpha_2 \rightarrow 0$ or $\beta \rightarrow 0$, the zero-flux Sherwood number or shape factor decreases from unity to zero. For large rates of mass transfer, the driving force also deviates significantly from the ideal 1-D solution, being lower for injection and higher for suction. The results of this study suggest that while there is not much change in the m distribution at the symmetry plane, compared to the 1-D solution, lateral variation in mass fraction m can vary for low values of the diffusion layer aspect ratio α_2 and/or blockage ratio β .

Conjugate mass transfer may be reasonably characterized from the mass transfer correlations for channels and diffusion layers. Since in normal fuel cells the blowing parameter generally falls well within the range $-1 \leq b \leq 1$, the driving force thus conforms well to an exponential distribution. The overall driving force may therefore be computed from known values of Sh_1^* , Sh_2^* , β , Γ_{eff}/Γ and b . This may be used to compute wall mass fractions from bulk values, necessary for electrochemical calculations. Thus mass transfer correlations reduce to essentially a universal form regardless of the particular details of the actual fuel cell design.

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Nomenclature

- A = area (m^2)
- D = diffusion coefficient (m^2/s)
- D_h = hydraulic diameter (m)
- F = Faraday's constant, 9.6487×10^7 (C/kmol)
- g = mass transfer conductance ($kg/m^2 s$)
- H = height (m)
- i'' = current density (A/m^2)
- J'' = superficial diffusion flux ($kg/m^2 s$)
- j'' = diffusion flux, interstitial diffusion flux ($kg/m^2 s$)
- k = permeability (m^2)
- M = molecular weight ($kg/kmol$)
- m = mass fraction (kg/kg)
- $\dot{m}''$ = mass flux ($kg/m^2 s$)
- p = pressure (Pa)
- U = superficial velocity (m/s)
- R = gas constant, 8.3144×10^3 J/kmol K
- T = temperature (K)
- u = interstitial velocity (m/s)

Table 2 Simplified procedure for calculation of overpotentials and limiting current density for a PEMFC.

		Cathode (air)				Anode (fuel)			
		H ₂ O	O ₂	N ₂	Σ	H ₂	H ₂ O	Σ	
1	x_b	1.00×10^{-1}	1.00×10^{-1}	8.00×10^{-1}	1.00	9.50×10^{-1}	5.00×10^{-2}	1.00	
2	M_s [kg/mol]	18	32	28	M_a [kg/mol]	2	18	M_f [kg/mol]	
3	x_b^s [M]	1.80	3.20	2.24×10^1	27.4	1.90	9.00×10^{-1}	28	
4	m_b	6.57×10^{-2}	1.17×10^{-1}	8.18×10^{-1}	1.00	6.79×10^{-1}	3.21×10^{-1}	1.00	
5	i'' [A/m ²]	1.00×10^4	1.00×10^4	1.00×10^4		1.00×10^4	1.00×10^4		
6	F	9.65×10^7	9.65×10^7	9.65×10^7		9.65×10^7	9.65×10^7		
7	n	2	4		m_2'' [kg/m ² s]	2	2	m_2'' [kg/m ² s]	
8	m_i'' [kg/m ² s]	1.87×10^{-3}	-8.29×10^{-4}	0.00	1.04×10^{-3}	-1.04×10^{-4}	-9.33×10^{-4}	-1.04×10^{-3}	
9	m_i	1.80	-8.00×10^{-1}			1.00×10^{-1}	9.00×10^{-1}		
10	Sh_1	2.71	2.71		m_1'' [kg/m ² s]	2.71	2.71	M_1'' [kg/m ² s]	
11	Sh_2	3.80×10^{-1}	3.80×10^{-1}		2.07×10^{-3}	3.80×10^{-1}	3.80×10^{-1}	-2.07×10^{-3}	
12	ρ [kg/ms]	2.94×10^{-1}	5.53	4.83	4.45	2.08×10^{-1}	2.94×10^{-1}	2.13×10^{-1}	
13	D [m ² /s]	6.52×10^{-6}	6.09×10^{-6}			3.89×10^{-5}	3.89×10^{-5}		
14	Γ [kg/ms]	2.90×10^{-5}	2.71×10^{-5}			8.27×10^{-6}	8.27×10^{-6}		
15	Γ_{eff} [kg/ms]	1.03×10^{-5}	9.57×10^{-6}			2.92×10^{-6}	2.92×10^{-6}		
16	g_1^s [kg/m ² s]	7.86×10^{-2}	7.34×10^{-2}			2.24×10^{-2}	2.24×10^{-2}		
17	g_2^s [kg/m ² s]	1.56×10^{-2}	1.46×10^{-2}			4.45×10^{-3}	4.45×10^{-3}		
18	b_1	2.64×10^{-2}	2.82×10^{-2}			-9.24×10^{-2}	-9.24×10^{-2}		
19	b_2	6.65×10^{-2}	7.12×10^{-2}			-2.33×10^{-1}	-2.33×10^{-1}		
20	b	9.29×10^{-2}	9.94×10^{-2}			-3.25×10^{-1}	-3.25×10^{-1}		
21	B_1	2.67×10^{-2}	2.86×10^{-2}			-8.83×10^{-2}	-8.83×10^{-2}		
22	B_2	6.87×10^{-2}	7.38×10^{-2}			-2.08×10^{-1}	-2.08×10^{-1}		
23	B	9.73×10^{-2}	1.05×10^{-1}			-2.78×10^{-1}	-2.78×10^{-1}		
24	B_{lim}		1.46×10^{-1}				-3.57×10^{-1}		
25	b_{lim}		1.36×10^{-1}				-4.42×10^{-1}		
26	i_{lim}'' [A/m ²]		1.37×10^4				1.36×10^4		
27	m_1	1.11×10^{-1}	9.13×10^{-2}	7.98×10^{-1}	1.00	7.35×10^{-1}	2.65×10^{-1}	1.00	
28	m_2	2.19×10^{-1}	3.00×10^{-2}	7.50×10^{-1}	1.00	9.01×10^{-1}	9.89×10^{-2}		
29	m_2/M	1.22×10^{-2}	9.39×10^{-4}	2.68×10^{-2}	3.99×10^{-2}	4.51×10^{-1}	5.49×10^{-3}	4.56×10^{-1}	
30	x_2	3.05×10^{-1}	2.35×10^{-2}	6.71×10^{-1}	1.00	9.88×10^{-1}	1.20×10^{-2}	1.00	
31	η [V]	-1.17×10^{-2}	-1.52×10^{-2}			4.10×10^{-4}		-1.47×10^{-2}	

W = width (m)
 x = mole fraction
 y = displacement (m)

Greek Symbols

α_i = aspect ratio, H_i/W_i
 β = blockage factor, W_1/W_2
 Γ = exchange coefficient (kg/ms)
 γ = interstitial exchange coefficient (kg/ms)
 ε = volume fraction
 η = concentration overpotential
 μ = dynamic viscosity (kg/ms)
 ρ = density (kg/m³)
 σ = conductivity (S/m)
 τ = tortuosity
 Φ = potential (V)

Nondimensional Numbers

B = mass transfer driving force
 b = blowing parameter
 Pe = Peclet number
 Re = Reynolds number
 Sh = Sherwood number, shape factor

Superscripts

$*$ = zero mass transfer, previous iteration
 $'$ = unit length
 $''$ = unit time

Subscripts

b = bulk
 eff = effective

lim = limiting
 p = in-cell
 t = transformed substance
 w = wall
 ∞ = external

Appendix: Sample Calculations

The sample calculations are for a typical PEMFC for which the following conditions are presumed: $W_1=H_1=1$ mm, $W_2=2$ mm, $H_2=0.25$ mm, $\varepsilon=0.5$. Hence, $\alpha_1=1$, $\alpha_2=1/8$, and $\beta=1/2$. Table 1 illustrates the calculation procedure. (1) The cathodic volume (mole) fractions for air are presumed as follows: $x_{H_2O}=0.1$, $x_{O_2}=0.1$, $x_{N_2}=0.8$; on the anode side the fuel is presumed to be $x_{H_2}=0.9$, $x_{H_2O}=0.05$, in the bulk. For the latter, it has been presumed that electro-osmotic drag results in exactly one H₂O molecule being dragged across the membrane for every H₂ molecule consumed by the reaction. The products of the mole fractions and (2) the molecular weights are summed to obtain (3) the mixture molecular weights, M_a and M_f according to Eq. (33). Thus, (4) the bulk mass fractions are computed using Eq. (32). Given (5) a presumed value of $i''=10,000$ A/m², (6) Faraday's constant F , and (7) the stoichiometric constants n , (8) the mass flow rates of the individual species may readily be computed by means of Faraday's law

$$\dot{m}_i'' = \pm \frac{Mi''}{1000nF} \quad (A1)$$

These are summed to obtain $\dot{m}_2''$ at the anode and the cathode. (9) The transferred-substance states are then computed from Eq.

(5). Values of (10) Sh_1^* and (11) Sh_2^* are obtained from the correlations for the given geometry, as shown in Figs. 3 and 9, respectively.

The exchange coefficients are computed from (12) the mean density and (13) the diffusion coefficients. The latter are evaluated at temperature T and pressure p , based on the recommendation of Cussler [20]

$$D_{ij}(T, p) = D_{ij}(T_0, p_0) \frac{p_0}{p} \left(\frac{T}{T_0} \right)^{1.75} \quad (A2)$$

Reference values were obtained from the NIST database.¹ Values given in Table 2 are estimated assuming the fuel to be at 3 atm, the air at 5 atm and the operating temperature to be 80°C. Water is assumed to be in the form of saturated steam. (14) The exchange coefficients Γ are thus obtained. Since $\Gamma_{H_2-H_2O}$ is a minimum, this will result in the largest magnitude in the blowing parameter b . (15) Γ_{eff} is then estimated using the Bruggeman assumption [21]

$$\frac{\Gamma_{eff}}{\Gamma} = \varepsilon^{3/2} \quad (A3)$$

so $\Gamma_{eff}/\Gamma = 0.3536$. (16) g_1^* and (17) g_2^* are estimated from Sh_1^* and Sh_2^* , respectively.

Values of at the blowing parameters (18) b_1 (19) b_2 , and (20) b are then computed using Eqs. (11) and (28). The reader will note that for the anode side; if there were no electro-osmotic drag a value of $b = -0.0332$ would correspond to $i'' = 10,000 \text{ A/m}^2$ with $m_i = 1$ for H_2 and $m_i = 0$ for H_2O for the fuel. However, electro-osmotic drag could increase this by up to a factor of 10, i.e., $b = -0.332$, with $m_i = 0.1$ for H_2 and $m_i = 0.9$, as indicated in Table 2. Thus, although $|b| < 1$, it is not by an order of magnitude, due to the osmotic drag of H_2O . Because $|b| < 1$, the driving forces (21) B_1 , (22) B_2 and (23) B may be obtained from the 1-D exponential theory (Eq. (14)). (24) The limiting driving force $B_{lim} = m_b/m_i$ is used to compute (26) b_{lim} and (27) trial values of i''_{lim} computed for each species, by means of Faraday's law. The minimum computed value of i''_{lim} is the rate limiting factor. It is apparent that for this PEMFC, a limiting current of 1370 A/m^2 would occur on the cathode side due to oxygen starvation, well before water transport at the anode becomes a limiting factor, and the membrane would dry out. Since i''_{lim} is an average value, a local limiting current density will actually occur sooner. Wall mass fractions at (27) the channel and (29) the diffusion layer may be obtained from Eq. (31) and hence (30) wall mole fractions, as above. Finally, (31) the concentration overpotentials for each species are computed

according to Eq. (34) from the wall and bulk mole fractions. These must be summed to obtain the overall potential losses. For this PEMFC, the majority of the concentration polarization is on the cathode side. However, the reader will note that if the bulk H_2O mole fraction were reduced from 5% on the anode side, dry-out of the membrane would occur at a much lower current density. The reader will note that the osmotic drag will almost certainly be reduced by back-diffusion and hence the blowing parameter will be smaller than that given here.

This PEMFC problem is an idealization and has been presented to illustrate the mass transfer calculation procedure. Other aspects, such as membrane protonic conductivity, multi-phase flow, and streamwise variation in bulk values will also play a part.

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