Influence of rib spacing in proton-exchange membrane electrode assemblies

A. C. WEST
Columbia University, Department of Chemical Engineering, Materials Science, and Mining Engineering, New York, NY 10027, USA

T. F. FULLER
International Fuel Cells, South Windsor, Connecticut 06074, USA

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A two-dimensional design analysis of a membrane-electrode assembly for a proton-exchange membrane fuel cell is presented. Specifically, the ribs of the bipolar plates restrict the access of fuel and oxidant gases to the catalyst layer. The expected change in cell performance that results from the partial blocking of the substrate layer is studied by numerical simulation of the oxygen electrode and the membrane separator. The effects of rib sizing and the thickness of the gas-diffusion electrode on the current and water distributions within the cell are presented. For all of the cases considered, the two-dimensional effect only slightly alters the half-cell potential for a given applied current but has a significant influence on water management.

Concentrated solution theory with variable transport properties is used in the membrane electrolyte to solve for the electrical potential and local water content. The Stefan–Maxwell equations are used in the gas-diffusion electrode to determine the local mole fractions of nitrogen, oxygen and water vapour.

A control-volume formulation is used for the resolution of the coupled nonlinear differential equations. One advantage of the control-volume approach over finite-difference methods is the relative ease in which internal boundary points in fuel-cell and battery models are handled. This and other advantages are briefly discussed.

List of symbols

\( a \quad \text{specific interracial area (m}^{-1}\) \)
\( A_k \quad \text{kinetic parameter defined by Equation 19 (kA m}^{-2}\) \)
\( c \quad \text{concentration (mol m}^{-3}\) \)
\( d_k^e \quad \text{coefficient in Equation 14} \)
\( D \quad \text{diffusion coefficient (m}^2\text{s}^{-1}\) \)
\( f_{i,k}^c \quad \text{coefficient in Equation 14} \)
\( F \quad \text{Faraday's constant (96 487 C equiv}^{-1}\) \)
\( h \quad \text{mesh spacing (m)} \)
\( i \quad \text{current density in electrolyte (A m}^{-2}\) \)
\( i_o \quad \text{exchange current density (A m}^{-2}\) \)
\( I \quad \text{superficial current density (A m}^{-2}\) \)
\( L_m \quad \text{thickness of membrane (m)} \)
\( L_s \quad \text{thickness of substrate (m)} \)
\( L_y \quad \text{thickness of rib (m)} \)
\( M \quad \text{molecular weight (g mol}^{-1}\) \)
\( N_i \quad \text{flux of species } i \text{ (mol m}^{-2}\text{s}^{-1}\) \)
\( n \quad \text{number of electrons transferred} \)
\( p \quad \text{pressure (Pa)} \)
\( R \quad \text{universal gas constant (J mol}^{-1}\text{K}^{-1}\) \)
\( R_h \quad \text{relative humidity} \)
\( R_i \quad \text{reaction state of species } i \text{ (mol m}^{-3}\text{s}^{-1}\) \)
\( s_i \quad \text{stoichiometric coefficient} \)
\( T \quad \text{temperature (K)} \)

\( V \quad \text{cell potential (V)} \)
\( x \quad \text{molar fraction of gas, and distance normal to membrane face (m)} \)
\( y \quad \text{distance (m)} \)

\( \alpha \quad \text{diffusion coefficient (J mol}^{-2}\text{m}^{-1}\text{s}^{-1}\) \)
\( \sigma_{e} \quad \text{weighting factor} \)
\( \beta_{e} \quad \text{weighting factor} \)
\( \Delta x \quad \text{element size in x-direction (m)} \)
\( \Delta y \quad \text{element size in y-direction (m)} \)
\( \Phi \quad \text{potential of electrolyte (V)} \)
\( \varepsilon \quad \text{porosity or numerical error} \)
\( \kappa \quad \text{conductivity of electrolyte (S m}^{-1}\) \)
\( \lambda \quad \text{dimensionless water concentration in membrane (moles water/mole sulfonate group)} \)
\( \rho \quad \text{membrane density (kg m}^{-3}\) \)
\( \sigma_{AB} \quad \text{characteristic length (m)} \)
\( \omega_{w} \quad \text{mass fraction of water} \)
\( \Omega_{AB} \quad \text{diffusion collision integral} \)
\( \xi \quad \text{transport number of water} \)
\( \mu \quad \text{chemical potential, J mol}^{-1}\) 

Subscripts

\( e \quad \text{cast face} \)
1. Introduction

The design of flow fields for fuel and oxidant feeds of a proton-exchange membrane (PEM) fuel cell is considered. The ribs of the bipolar plates restrict the access of fuel and oxidant gases to the catalyst layer, affecting the current distribution in the cell. The expected change in cell performance that results from the partial blocking of the substrate layer is an important factor in the design of a fuel-cell system. The sizing of the ribs and the thickness of the substrate also affect water distribution within a PEM cell. Perfluorinated ionomer membranes require absorbed water to maintain sufficient electrical conductivity for practical use, and it is vital to manage the water content in the solid-polymer electrolyte. From the inception of solid-polymer-electrolyte fuel cells, water transport was recognized as a problem. Water motion is caused by the movement of hydrogen ions, which is proportional to the current. High current densities can result in the transport of water away from the anode-membrane interface at a rate that is greater than the rate at which it can be restored by diffusion, or transported from a humidified gas stream.

Modelling is an important tool in the design and optimization of batteries and fuel cells. The numerical solution to the coupled, nonlinear, partial differential equations is usually carried out by means of a finite-difference formulation, using a block, tridiagonal matrix algorithm (TDMA), normally based on the Thomas method. For the numerical simulation of fuel cells and batteries, there are two shortcomings associated with the standard, Taylor series-based finite-difference approach.

First, inherent in any battery or fuel-cell system are interior boundaries separating distinct phases. For example, the interface between the electrolyte and the gas-diffusion electrode of a fuel cell forms a boundary for the gas and electrolyte phases, for which interior boundary conditions must be imposed. The standard finite-difference formulation of these interior boundary conditions results in block pentadiagonal matrices, which are more difficult to resolve than the tridiagonal matrices. Various schemes, including the employment of pentadiagonal matrix solvers, have been used to circumvent this problem [1, 2]. An alternative is to use derivatives whose accuracy is only first order in the node spacing. Although this allows internal boundaries to be readily handled, the low accuracy of this method may give unsatisfactory convergence results.

Second, the standard finite-difference method does not rigorously conserve material (or momentum and energy). The amount of electrolyte in a battery, for instance, may increase with simulation time, clearly a nonphysical result. The control-volume formulation, sometimes called the finite-volume method, rigorously conserves material and handles easily interior boundaries. These two advantages of the control-volume approach will become even more important as two or three-dimensional numerical simulations become prevalent.

The objectives of this paper are to review the control-volume formulation and to apply it to a two-dimensional problem of interest for fuel-cell modelling.

2. Control-volume formulation

The control-volume approach has been used extensively in heat-transfer and fluid-flow simulations [3], but to a lesser degree in the modelling of battery and fuel-cell systems. Recently, Fiard and Herbin [4] compared a control-volume approach to a finite-element method for the simulation of a solid-oxide fuel cell. They found that the control-volume technique was computationally superior to the finite-element approach and somewhat easier to implement. The control-volume method, or integrated element approach, has been used in conjunction with the finite-difference method to handle interior boundaries in fuel-cell [5] and battery modelling [6]. However, it is more logical to use the control-volume approach across the entire solution domain, as was done by Pollard and Newman [7, 8]. The benefits and details of their approach are not given in their paper.

The control-volume concept is simple — the differential form of the material balance is replaced with an integrated form. Consider one-dimensional transport in the element shown in Fig. 1. At steady state, a shell mass balance is written as

\[
\text{rate of mass in} - \text{rate of mass out} + \text{rate of production} = 0
\]

or on a unit area basis,

\[
N_A \left( x - \frac{h}{2} \right) - N_A \left( x + \frac{h}{2} \right) + R_A h = 0 \tag{1}
\]

\(N_A\) is the flux of species A, \(R_A\) is the homogenous production rate, and \(h\) is the thickness of the element. Typically, after making the balance for a shell of finite

![Fig. 1. A control volume used in the integrated-element approach.](image-url)

Fluxes are evaluated at the faces between node points. In this approach, material is rigorously conserved.