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Mass transfer formulation for polymer electrolyte membrane fuel cell cathode

Steven B. Beale

Institute of Energy and Climate Research, IEK-3, Forschungszentrum Jülich GmbH, 92425 Jülich, Germany

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ABSTRACT

A standard mechanical engineering mass transfer analysis is adapted to obtain performance calculations for the cathode of a typical polymer electrolyte membrane fuel cell. Mathematical details are provided and sample calculations performed, based on a number of simplifying assumptions. The relative advantages of low and high-mass transfer formulations are critically appraised and compared to a highly-simplified method.

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Introduction

It is popular within some elements of the fuel cell modelling community to consider accounting for diffusion losses with expressions with the following generic form,

$$\dot{m}_i'' = g(y_e - y_b), \quad (1)$$

where the rate-of-reaction of species *i* (oxygen), \dot{m}_i'' kg/(m²·s), is given by a Butler-Volmer equation or the like. Phenomenological models for mass transfer mechanisms are typically invented to enumerate the mass transfer coefficient or conductance, *g*, in Eq. (1), which may easily be written in a volumetric form, as opposed to per unit area, and is often cast in spherical polar coordinates for idealised particles, or agglomerations of such particles.

The molar form of Eq. (1),

$$\dot{n}_i'' = k(x_e - x_b), \quad (2)$$

is also widely found in the electrochemical literature, and is to be considered equivalent [1]. The purpose of this paper is to consider the class of formulation exemplified by Eq. (1), investigate the range of circumstances under which it is realistic, and to propose some modifications and extensions where necessary.

In a previous work [2], the present author identified limitations of Eq. (1) when applied to problems where gases are employed as fuel and oxidant. It is generally accepted that the range of validity is confined to two situations: (i) very dilute mixtures and (ii) chemical catalysis with no net mass transfer at the boundary. The reader is referred to [3] for further details.

Consider the idealised case shown in Fig. 2 where it is assumed that the cathode is in the form of a porous media, and that the solid electrode material is surrounded by a liquid, or liquid-like, water/Nafion® film, through which oxygen is transported. Water also is transferred either (a) into the liquid film and/or as vapour in the gas phase. For mass transfer in porous media it is common to employ volume-averaging techniques, and Fig. 3 illustrates schematically the volume-

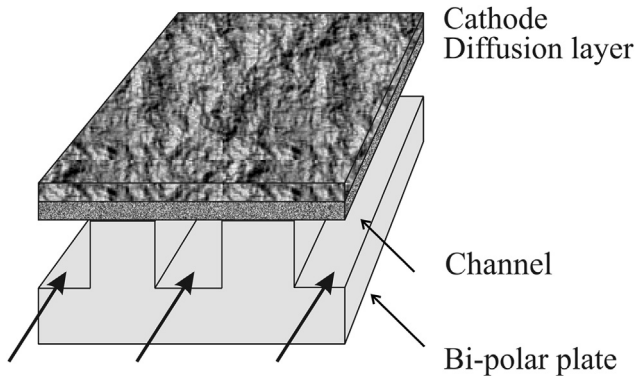
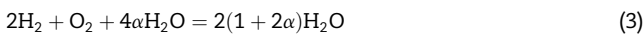


Fig. 1 – Typical PEM Cathode Assembly (not to scale).

averaged values of the bulk, wall, and interfacial values of the mass fraction which may be considered as locally 1-D for the purpose of the analysis. Let y_e denote the mass fraction of the dissolved oxygen in the liquid film near the electrode wall, y_l the value in the film near to the liquid–gas interface, y_g the oxygen mass fraction in the gas-phase near to the liquid–gas interface and y_b the bulk value in the gas free stream. One further concept is introduced, namely the notion of the transferred-substance, or T-state, value denoted by y_t . The unfamiliar reader is referred to [3–5] and below, for details.

Fig. 3 represents the very simplest possible idealisation of a cathode of a polymer electrolyte membrane fuel cell (PEMFC) for the purpose of the analysis. The air layer transfers oxygen to the liquid film, and thence to the solid electrode interface. The overall reaction at the electrode assembly may be written,



where the drag coefficient, α , is the net number of water molecules per proton emerging at the cathode: In a PEMFC, electro-

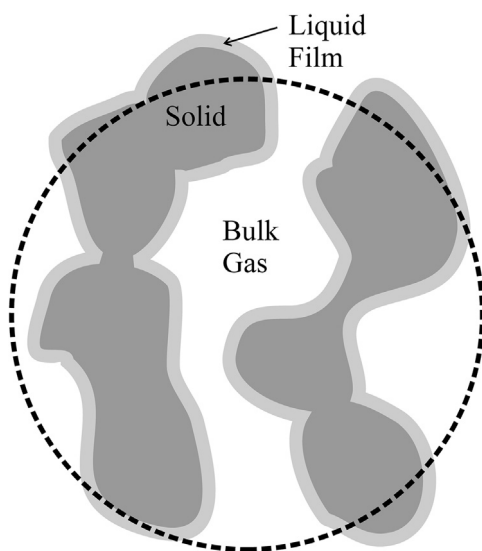


Fig. 2 – Schematic of porous media, illustrating volume-averaging process.

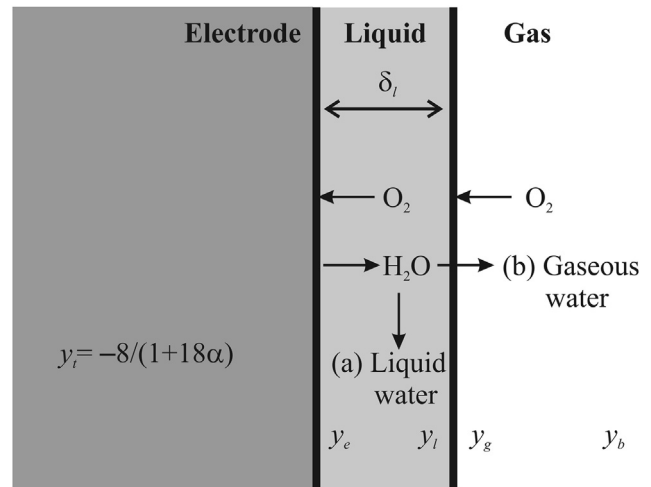


Fig. 3 – Unravalled cathode showing nomenclature.

osmotic forces drag n_d water molecules through the membrane with each proton. Electro-osmotic drag is modified (reduced) by back diffusion from the cathode to the anode, and also by a convective flux in the event of there being a significant pressure gradient between the two electrodes, to yield a net value α , typically less than 1. Dai et al. [6] review the experimentally determined values, and the results of calculations from mathematical models for water balance in PEMFC membrane electrode assemblies, and present ranges of values for both n_p and α .

A mass balance may be written as follows,

$$\dot{m}'' = \left(\dot{m}''_{\text{H}_2} + \dot{m}''_{\text{H}_2\text{O}} \right)_{\text{anode}} = \left(\dot{m}''_{\text{O}_2} + \dot{m}''_{\text{H}_2\text{O}} \right)_{\text{cathode}} \quad (4)$$

$$(4 + 4\alpha \times 18)\text{kg} = -32\text{kg} + 2(1 + 2\alpha)18\text{kg}$$

The T-state value for the oxygen phase is defined as;

$$y_t = \dot{m}''_{\text{O}_2} / \dot{m}'' \quad (5)$$

so that $y_t = -8/(1+18\alpha)$, as shown in Fig. 4. The water T-state is just $1 - y_t$. Oxygen mass transfer is generally considered as being an important and potentially rate-limiting factor in the

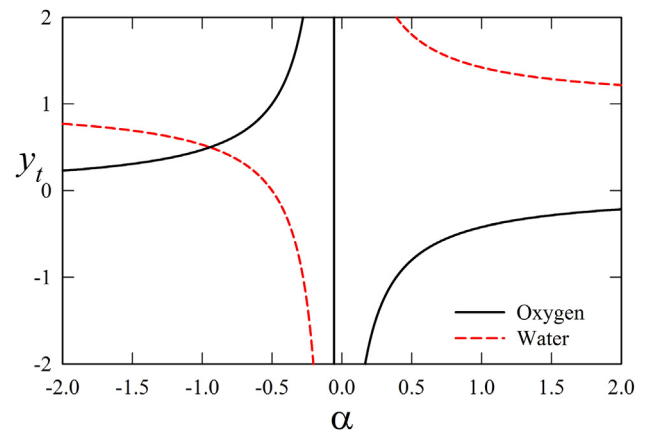


Fig. 4 – Transferred-state values of oxygen and water as a function of the net water drag coefficient, α

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