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Full Length Article

Accurate analytical model for determination of effective diffusion coefficient of polymer electrolyte fuel cells by designing compact Loschmidt cells

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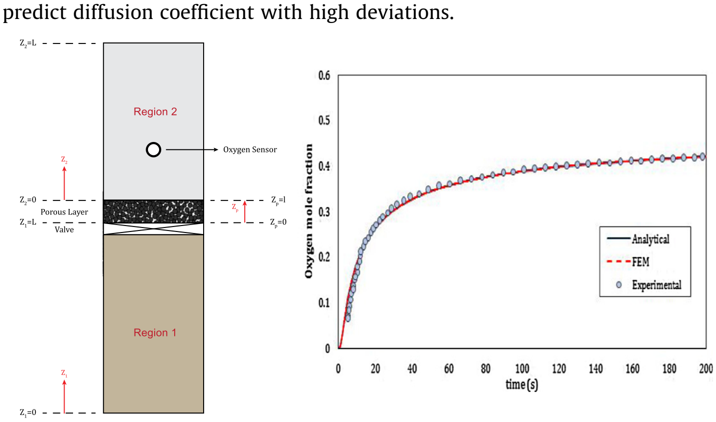
HIGHLIGHTS

- An analytical model is presented for study of diffusion in composite systems.
- The model can be used to design more compact and cheaper Loschmidt cells.
- Results are well matched with experimental measurements and finite element method.
- The conventional models can show poor predictions in later times and short cells in comparison with the new proposed model.

GRAPHICAL ABSTRACT

Effective diffusion coefficient is an important parameter which needs to be determined in different fields of study, such as cathode catalyst layers of PEM fuel. For this purpose, a Loschmidt diffusion cell can be used. When a porous medium is placed in Loschmidt apparatus, the effective gas diffusion coefficient (EGDC) of this section must be correlated by diffusion coefficient in absence of a porous medium.
In the previous researches studying the Loschmidt diffusion cell, a simplifying infinite-length assumption was used in the analytical solution. Therefore, the solution is only applicable for a short time range, and this can result in high error. In order to overcome this challenge, the length of cell should be quite long. This requirement is not experimentally and economically easy to achieve.
In this study, a new analytical solution is proposed by applying Fick's second law and separation of variables technique. This model does not use simplifying assumptions such as infinite length and equivalent diffusivity coefficient. The results of the new analytical solution are verified with the experimental measurements, as well as numerical finite element simulation. In order to analyze the reliability of previous methods, a new characteristic time is defined based on diffusion wave propagation in the system. Finally, a sensitivity analysis on thickness of porous media and EGDC is conducted and it is shown that previous models can predict diffusion coefficient with high deviations.



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Nomenclature

A	constant
B	constant
C	concentration
D	diffusion coefficient
D_{bulk}	binary diffusion coefficient
D_{eq}	equivalent diffusion coefficient
D_{eff}	effective diffusion coefficient
$D^{(e)}$	conductance matrix
erf	error function
erf^{-1}	inverse error function
$F_g^{(e)}$	nodal forcing function
j	mass flux
l	porous sample thickness
L	channel length
m	number of series terms
M	number of region
$M^{(e)}$	element capacitance matrix
N	norm
N_i	interpolation function
t	time
$T^{(e)}$	column matrix of element nodal concentration
Z	cell direction axis

Greek symbols

τ	characteristic diffusion time
β	constant of integration
ψ	space function
Γ	time function

Subscripts

1	region 1
2	region 2
3	region 3
f	fracture
m	matrix
max	maximum
min	minimum
R	ratio

1. Introduction

Polymer electrolyte membrane (PEM) fuel cells are considered as innovative, alternative and green energy technologies systems which can be integrated with traditional power sources as new candidates in transportation, stationary power systems, and portable devices [1].

In order to improve the efficiency of PEM fuel cells in comparison with traditional power sources, they are designed to operate at high current densities up to 1.5 A/cm^2 with the power in the range of 600 mW/cm^2 and even higher [2,3]. However, high current densities can result in an increase in loss due to mass transport. Therefore, it is essential to study the different parameters of the system such as transport coefficients comprehensively [3].

In order to estimate the binary and effective diffusion coefficients of two gases, based on transient method (time-dependent concentration boundary condition), a Loschmidt diffusion cell can be used [4,5]. A Loschmidt diffusion cell is an apparatus consisting of two chambers and a sliding gate which connects the top and bottom chambers. A special Oxygen sensor is embedded in top chamber, in order to measure the Oxygen concentration. The chambers are filled with different concentrations of gases, and diffusion takes place upon the removal of the gate. The changes in concentration with time can be used to determine the diffusion coefficient [6,7].

Several studies have focused on theoretical modeling of binary and effective gas diffusion coefficient through porous media in fuel cells [6,8]. Göll and Piesche [9] presented a computational model based on a theory of multi component gas transport in porous media, which can be used for investigations in macroscopic scale. In order to validate their model, they simulated an isothermal diffusion problem in a Loschmidt cell by using mass transfer model; however, the results of this model were presented in numerical simulations.

The Loschmidt diffusion cell can also be used for determination of the effective diffusion coefficients of cathode catalyst layers of PEM fuel cells. Shen et al. [10] measured the effective diffusion coefficient of dry gas (O_2–N_2) in gas diffusion layers by an in-