Cell performance modeling of direct methanol fuel cells using proton-exchange solid electrolytes

S. Jessie Lue\textsuperscript{1}, Bo Yan Wang\textsuperscript{2}, Hun Kai Lin\textsuperscript{2}, and K.P.O. Mahesh\textsuperscript{3}

Department of Chemical and Materials Engineering, Chang Gung University, Kwei-shan, Taoyuan 333, Taiwan

Tel: (03)2118800 ext.5489; Email: jessie@mail.cgu.edu.tw

\textsuperscript{1}Professor, \textsuperscript{2}Graduate student, \textsuperscript{3}Post doctor

In the past, some works have been devoted on predicting the model to better understand the phenomena arising within the DMFC using various solid polymer electrolyte membranes. We have modified the Kulikovsky model to improve the DMFC cell performance. The proposed model is to improve the effective diffusion coefficients of reactants (methanol and oxygen) in the gas diffusion layers and to further estimate the limiting current densities. We have successfully used this model to predict the cell performance at different operating temperature and feed concentration. As well as we have used different polymer electrolytes viz., Nafion117, Nafion115, sulfonated poly(phthalazinone ether ketone), sulfonated poly(ether ether ketone), and highly porous PTFE membrane as the framework structure and dip it in sulfonated poly[styrene-b-(ethylene-r-butylene)-b-styrene] (sSEBS) solution to prepare a sSEBS/PTFE composite membrane to compare the cell performance of these electrolytes. Further, the DMFC performance obtained by this model was validated with experimental results, operating at 30 – 80°C with 1-5 M methanol feed.

Fig. 1. Modeling and experimental curve for Nafion117 at 70°C.
This modified model was able to predict the effect of methanol concentration on the cell performance. In contrary, the conventional Kulikovsky model failed to estimate the cell voltage for methanol concentration over 3M. Even with 1M and 2M methanol feeds, this model outperformed Kulikovsky model by 9.4–13.7%. The simulation model provides a valuable prediction tool for researchers and can save time and cost on fuel cell tests, particularly in reducing the usage of pricey catalysts and electrolytes.
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Chang Gung University, R.O.C.
Wang, Bo Yan

Outline

- Introduction of fuel cells
- sSEBS (sulfonate Poly(styrene-ethylene-butylene-styrene)) as proton-exchange electrolytes
  1. Crosslinked sSEBS
  2. PTFE/sSEBS composite
- Performance of DMFC
- DMFC mathematical model
- Concluding remarks
Green Energy

1. Fuel cells
2. Solar cells
3. Biomass
4. Aero generator
5. Geothermic

Direct methanol fuel cells

Anode

\[ \text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2(g) + 6\text{H}^+ + 6\text{e}^- \]

Cathode

\[ 2/3\text{O}_2 + 6\text{H}^+ + 6\text{e}^- \rightarrow 3\text{H}_2\text{O} \]
Proton Exchange Membrane Fuel Cell

1. Inexpensive
2. Sufficient conductivity
3. High thermal stability
4. Low methanol permeability

Crosslinked sSEBS
PTFE/sSEBS composite membrane

Framework

Porous PTFE  Dipped  vacuumed  sSEBS solution  Vacuum dry at 120°C, 6Hr

fig. 1 porous PTFE cross section  fig. 2 PTFE/sSEBS cross section

Proton conductivity and methanol permeability

Selectivity  \( \beta = \sigma / P \)

\( \beta = 5585 \quad \beta = 5201 \quad \beta = 3846 \)

Fig. 3. MeOH permeability and conductivity.
Performance of **PTFE/sSEBS** at 1M MeOH and at various temperatures

Fig. 4. DMFC’s V-I curves.

Fig. 5. DMFC’s P-I curves.

Performance of **PTFE/sSEBS** at 60°C and various MeOH concentrations

Fig. 6. DMFC’s V-I curves.

Fig. 7. DMFC’s P-I curves.
Performance of DMFC with various membrane

Fig. 8. DMFC’s V-I curves at 1M MeOH and 60°C.

Fig. 9. DMFC’s P-I curves at 1M MeOH and 60°C.

Modeling of DMFC performance using PTFE/sSEBS electrolyte

Fig. 10. Prediction (solid lines) and experimental of DMFC using sSEBS electrolyte at 30°C and 60°C with 1M.
Modeling of Nafion Performance at 1M MeOH

Fig. 11. Prediction and experimental I-V curves at various temperatures.

Fig. 12. Prediction and experimental P-I curves at various temperatures.

Modeling of performance of sPEEK electrolyte

Fig. 13. Prediction (solid lines) and experimental of DMFC using sPEEK electrolyte.
Conclusion

◆ sSEBS is a promising electrolyte material for DMFC.

◆ Performance of G-sSEBS (83mW/cm²), PTFE/sSEBS (80mW/cm²) were better than Nafion117 (70.6mW/cm²).

◆ Modified Kulikovsky’s model could predict cell performance, even at high methanol concentrations.

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Modified Kulikovsky’s model

\[ V = E^0 - \eta_a - \eta_{\Omega} - \eta_c \]

\[ \eta_a = b_a \ln\left(\frac{i}{i_{sa}}\right) - b_a \ln(1 - \frac{i}{i_{sa}}) + b_a \ln(1 - \mu) \]

\[ \eta_{\Omega} = \frac{\alpha L}{\sigma} \]

\[ \eta_c = b_c \ln\left(\frac{i}{i_{sc}}\right) - b_c \ln\left(1 - \frac{i}{i_{sc}}\right) - R_c \]

\[ \mu = \frac{\beta}{L} \frac{L_{ba}}{D_{ba}} \]

\[ i_{fa} = 6 F \frac{D_{ba}}{L_{ba}} \]

\[ D_{MW} = (D_{MW} x_M + D_{MW} x_W) \alpha \]