Chapter 07.00B

Physical Problem for Integration Chemical Engineering

Although a fuel cell provides DC electricity like an ordinary battery, it differs from an ordinary battery from the fact that its fuel source is externally supplied and as long as the fuel is being supplied, the fuel cell can in theory run continuously without needing a recharge. The two electrochemical reactions in a fuel cell occur at the electrodes (or poles) to which reactants are continuously fed. The reaction at the negative electrode (anode) is maintained by supplying a fuel such as hydrogen or methanol, whereas the positive electrode (cathode) reaction is maintained by the supply of oxygen or air. The two electrodes (anode and cathode) are separated by a proton conducting membrane – polymer electrolyte membrane (PEM).

A schematic diagram showing the operating principles of fuel cell that utilizes methanol as fuel, i.e., a Direct Methanol Fuel Cell (DMFC) is shown below.

![Schematic diagram of a Direct Methanol Fuel Cell (DMFC)](Diagram)

**Figure 1.** Direct methanol fuel cell

DC current is produced in the DMFC when methanol is electrochemically oxidized at the anode electrocatalyst. The electrons produced from the oxidation reaction leave the anode and travel through the external circuit to the cathode electrocatalyst where they are consumed together with oxygen in a reduction reaction. The circuit is maintained within the cell by the conduction of protons in the electrolyte (PEM).
Because of ease of design and its ability to withstand high temperature and pressure operation, most fuel cells today use PEM such as Nafion™.

The overall reaction occurring in the DMFC is equivalent to the direct combustion of methanol:

\[
2\text{CH}_3\text{OH} + 3\text{O}_2 \rightarrow 4\text{H}_2\text{O} + 2\text{CO}_2
\]

One of the problems affecting the performance and hence commercialization of the direct methanol fuel cell (DMFC) is the depolarization of the oxygen reduction electrode caused by methanol cross-over. Depolarization as used here means that the presence of methanol limits the oxygen reduction and hence the amount of electricity produced. The exact role of methanol in limiting oxygen reduction can be inferred by understanding the physics and chemistry of the reaction. In an attempt to understand the mechanism of the depolarization process, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in our laboratory. A very simplified model [1] of the reaction developed suggests a functional relation of the form

\[
T = -\int_{x_1}^{x_2} \left( \frac{6.73x + 6.725 \times 10^{-8} + 7.26 \times 10^{-4} C_{me}}{3.62 \times 10^{-12} x + 3.908 \times 10^{-8} xC_{me}} \right) dx
\]

where

\[
T = \text{time in s}
\]
\[
x = \text{Concentration of oxygen, moles/cm}^3,
\]
\[
C_{me} = \text{Concentration of methanol, moles/cm}^3,
\]

The parameters [1] in the above equation are

\[
C_{me} = 5 \times 10^{-4} \text{ moles/cm}^3
\]

The initial concentration is

\[
x(t = 0) = 1.22 \times 10^{-6} \text{ moles/cm}^3
\]

QUESTIONS

1. Evaluate the time required for 50% of the initial oxygen concentration to be consumed in the fuel cell in the presence of methanol.

2. Repeat (a) in the absence of methanol (that is, \(C_{me} = 0\)). What can you infer from the result in (a) and (b)?

3. Plot time vs. oxygen concentration for the following concentrations of oxygen -
\[
x = [1.22, 1.20, 1.0, 0.8, 0.6, 0.4, 0.2] \times 10^{-6} \text{ moles/cm}^3\]
both in the presence and absence of methanol.

References

1. Itoe, R.N., Analysis of simultaneous oxygen reduction and methanol oxidation process in a direct methanol fuel cell, MS Thesis, Department of Chemical and Biomedical Engineering, Florida A&M University (1999).
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<td>Egwu Kalu</td>
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