CHAPTER 3 METHODOLOGY

The COMSOL Multiphysics program was used in this work to implement the mathematical model of direct methanol fuel cell (DMFC). This chapter describes a methodology to achieve this work. The procedures to complete each step of the methodology are briefly outlined.

3.1 Methodology

There are 6 work steps to be carried out in this work. Each step and its description is described below.

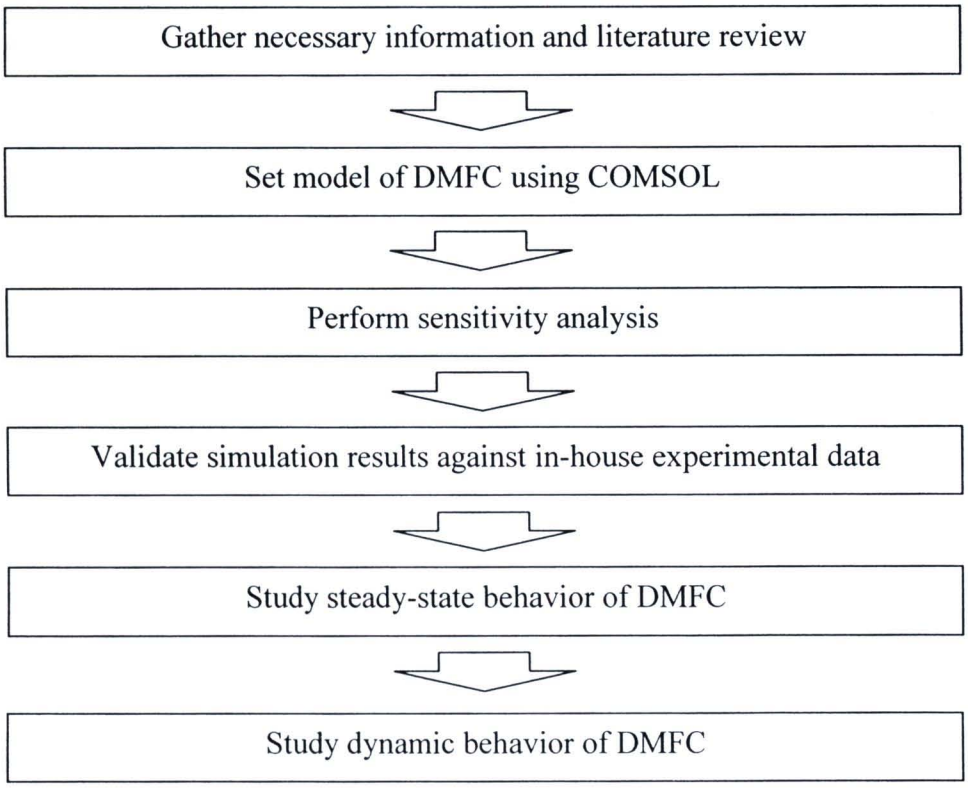

Figure 3.1 The methodology chart

3.1.1 Gather Necessary Information and Literature Review

First of all, the necessary information about the fuel cell process was gathered to first understand how the fuel cell works. The data were obtained from literature, handbooks and internet. The basic principles of fuel cell and equations can be collected from handbooks. The steady state and dynamic mass transport models of DMFC were taken from the literatures.

3.1.2 Set the Model of Direct Methanol Fuel Cell

The model of DMFC is a transient two-phase mass transport model. The model was implemented in COMSOL Multiphysics program. The model consists of species balance, overall mass balance of gas-and liquid-phase, electrochemical kinetics, and charge balance. The 11 major variables interested in this work are liquid methanol, methanol vapor, water vapor, and oxygen concentrations, anode and cathode liquid saturation, liquid pressure at anode region, gas pressure at cathode region, anode and cathode overpotentials, and surface coverage of CO.

3.1.3 Perform Sensitivity Analysis

Sensitivity analysis was performed in order to study the influences of the changing parameters on the simulation result. The parameters which affect the anode overpotential and cell voltage are reaction rate constant, transfer coefficient and exchange current density. Thus, these three parameters were individually varied to observe their trend.

3.1.4 Validate Simulation Result Against In-house Experimental Data

In this step, the simulation results which were anode overpotential and cell voltage were validated with in-house experimental data to ensure the model prediction effectiveness. If the model results correspond with experimental results, the next step can be done otherwise the sensitivity analysis must be repeated.

3.1.5 Study Steady-state Behavior of DMFC

After the anode overpotential and cell voltage match with experimental data, the other parameters namely, polarization losses, liquid saturation, methanol liquid concentration and oxygen concentration were studied at various current density. Moreover, the behavior of DMFC resulted from single-phase and two-phase models were compared with each other.

3.1.6 Study Dynamic Behavior of DMFC

The last step was studying the behavior of DMFC when the current density was suddenly changed. The simulation results such as cell voltage, anode and cathode overpotential, or concentrations of methanol, oxygen and water, were studied in terms of the dynamic behavior.