



National Library  
of Canada

Acquisitions and  
Bibliographic Services Branch

395 Wellington Street  
Ottawa, Ontario  
K1A 0N4

Bibliothèque nationale  
du Canada

Direction des acquisitions et  
des services bibliographiques

395, rue Wellington  
Ottawa (Ontario)  
K1A 0N4

Your file    *Voire référence*

Our file    *Notre référence*

## NOTICE

The quality of this microform is heavily dependent upon the quality of the original thesis submitted for microfilming. Every effort has been made to ensure the highest quality of reproduction possible.

If pages are missing, contact the university which granted the degree.

Some pages may have indistinct print especially if the original pages were typed with a poor typewriter ribbon or if the university sent us an inferior photocopy.

Reproduction in full or in part of this microform is governed by the Canadian Copyright Act, R.S.C. 1970, c. C-30, and subsequent amendments.

## AVIS

La qualité de cette microforme dépend grandement de la qualité de la thèse soumise au microfilmage. Nous avons tout fait pour assurer une qualité supérieure de reproduction.

S'il manque des pages, veuillez communiquer avec l'université qui a conféré le grade.

La qualité d'impression de certaines pages peut laisser à désirer, surtout si les pages originales ont été dactylographiées à l'aide d'un ruban usé ou si l'université nous a fait parvenir une photocopie de qualité inférieure.

La reproduction, même partielle, de cette microforme est soumise à la Loi canadienne sur le droit d'auteur, SRC 1970, c. C-30, et ses amendements subséquents.

**Simulation of the Proton Exchange Membrane Fuel Cell:  
Dynamic Modelling and an Environment**

**by Neil Keon**

**A thesis  
submitted to the School of Graduate  
Studies and Research of the University of Ottawa  
in partial fulfillment of the requirements of  
Master of Science in Systems Science**

**University of Ottawa**

**Ottawa, Ontario**

**Canada**

**October 17, 1995**

**© Neil Keon, Ottawa, Ontario, Canada, 1995**



National Library  
of Canada

Acquisitions and  
Bibliographic Services Branch

395 Wellington Street  
Ottawa, Ontario  
K1A 0N4

Bibliothèque nationale  
du Canada

Direction des acquisitions et  
des services bibliographiques

395, rue Wellington  
Ottawa (Ontario)  
K1A 0N4

Your file    Votre référence

Our file    Notre référence

The author has granted an irrevocable non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of his/her thesis by any means and in any form or format, making this thesis available to interested persons.

L'auteur a accordé une licence irrévocable et non exclusive permettant à la Bibliothèque nationale du Canada de reproduire, prêter, distribuer ou vendre des copies de sa thèse de quelque manière et sous quelque forme que ce soit pour mettre des exemplaires de cette thèse à la disposition des personnes intéressées.

The author retains ownership of the copyright in his/her thesis. Neither the thesis nor substantial extracts from it may be printed or otherwise reproduced without his/her permission.

L'auteur conserve la propriété du droit d'auteur qui protège sa thèse. Ni la thèse ni des extraits substantiels de celle-ci ne doivent être imprimés ou autrement reproduits sans son autorisation.

ISBN 0-612-11566-6

Canada



UNIVERSITÉ D'OTTAWA  
UNIVERSITY OF OTTAWA

## **ACKNOWLEDGEMENTS**

I would like to express sincere gratitude to a number of people for their assistance in the preparation of this thesis.

I am grateful to my supervisor, Dr. Tuncer I. Ören for his patience as I learned throughout the past year, and his many thoughtful suggestions concerning this project. I am appreciative of the time he spends thinking of his students.

I would like to thank Dr. Julio C.T. de Oliveira and Dr. Guenter Simader from ESTCO Energy Inc. of Ottawa. Their support and guidance has helped to make this thesis multidisciplinary, which is one of the goals of the Systems Science Programme.

I would like to thank Michel de Breyne for his generous assistance with portions of the programming.

Finally, I would like to thank my parents for their support, and for giving me an appreciation of the value of education.

## **TRADEMARK & COPYRIGHT ACKNOWLEDGEMENTS**

<b>ACSL</b>	<b>is a trademark of Mitchell &amp; Gauthier Associates (MGA) Inc.</b>
<b>Visual Basic</b>	<b>is a trademark of Microsoft Corporation</b>
<b>Gest and GestCell</b>	<b>are trademarks of Dr. Tuncer I. Ören</b>
<b>Microsoft Excel</b>	<b>is a trademark of Microsoft Corporation</b>
<b>Microsoft Windows</b>	<b>is a trademark of Microsoft Corporation</b>
<b>OLE 2.0</b>	<b>is a trademark of Microsoft Corporation</b>

## **ABSTRACT**

The proton exchange membrane fuel cell (PEMFC) is the focus of modeling and simulation efforts in order to better understand this technology and improve its design and operation. Simulated polarization curves for PEMFCs duplicate the observed performance of PEMFCs with varying degrees of success. In order for modelling and simulation to be more widely used in this field and elsewhere, effective tools must be made available for non-programmers to apply their knowledge to simulation problems.

GestCell (A modelling and simulation environment based on Gest) is a new modelling and simulation environment designed with non-programmers in mind, in particular scientists studying PEMFCs. A friendly graphical interface allows users who are knowledgeable in a non-programming field to enter information about a system into GestCell, which automatically constructs a Gest specification. The Gest specification is highly readable for the user, and the system is able to generate a C++ program with the specification in order to allow the user to carry out simulation with the model, with very little knowledge in the area of simulation. GestCell is very general in nature and could be used in a wide variety of fields. It has a great deal of potential to be a powerful modelling and simulation environment.

## LIST OF FIGURES

Figure 1. Possible Polarization curve for a PEMFC.....	11
Figure 2. Diagram of the dynamic processes occurring within the PEMFC.....	26
Figure 3. Outline of a Gest specification of a mathematical model and a simulation experiment.....	34
Figure 4. Overall Architecture of GestCell.....	41
Figure 5. Pointer structure attached to Gest specifications in GestCell.....	43
Figure 6. GestCell at start up.....	44
Figure 7. Opening an existing Gest Specification.....	45
Figure 8. GestCell interface in Excel®.....	46
Figure 9. Editing Dialog box displayed after pressing the Add toolbar button.....	48
Figure 10. Parameter set dialog box.....	50
Figure 11. Experiment specification dialog box.....	51
Figure 12. Output dialog box.....	52
Figure 13. Simulation dialog box.....	55
Figure 14. Gest specification of a pendulum model constructed using GestCell.....	57
Figure 15. Gest specification of pendulum model parameters, initial values and experiment.....	58
Figure 16. Top of output data generated using GestCell (pendulum model).....	59
Figure 17. Simulated partial pressures of feedstream gases in a PEMFC.....	61
Figure 18. Simulated cell voltage for a PEMFC.....	61

## LIST OF TABLES

Table 1. Types Of Fuel Cells.....	8
Table 2: Components Of Dynamic Model Of The Proton Exchange Membrane Fuel Cell (Pemfc) .....	28

## TABLE OF CONTENTS

ACKNOWLEDGEMENTS.....	i
TRADEMARK & COPYRIGHT ACKNOWLEDGEMENTS.....	ii
ABSTRACT.....	iii
LIST OF FIGURES.....	iv
LIST OF TABLES.....	v
1. INTRODUCTION.....	1
1.1 MOTIVATION.....	1
1.2 STRUCTURE OF THE THESIS.....	2
2. FUEL CELLS.....	4
2.1 GENERAL DESCRIPTION OF A FUEL CELL.....	4
2.2 TYPES OF FUEL CELLS.....	5
2.2.1 <i>The Alkaline Fuel Cell (AFC)</i> .....	5
2.2.2 <i>The Phosphoric Acid Fuel Cell (PAFC)</i> .....	6
2.2.3 <i>The Molten Carbonate Fuel Cell (MCFC)</i> .....	6
2.2.4 <i>The Solid Oxide Fuel Cell (SOFC)</i> .....	7
2.2.5 <i>The Proton Exchange Membrane Fuel Cell (PEMFC)</i> .....	7
2.3 ENERGY LOSSES WITHIN THE CELL.....	8
2.3.1 <i>Activation polarization</i> .....	9
2.3.2 <i>Ohmic polarization</i> .....	9
2.3.3 <i>Concentration polarization</i> .....	10
2.4 SURVEY OF MATHEMATICAL MODELS OF THE PEMFC.....	11
2.4.1 <i>Springer, et. al.</i> .....	11
2.4.2 <i>Bernardi &amp; Verbrugge</i> .....	13
2.4.3 <i>Fuller &amp; Newman</i> .....	13
2.4.4 <i>Nguyen and White</i> .....	14
2.4.5 <i>RMC Model</i> .....	15
2.5 SUMMARY OF STEADY STATE MODELS AND SIMULATION.....	16
3. DYNAMIC MODELLING OF THE PEMFC: ISSUES.....	17
3.1 TRANSPORT PHENOMENA PROCESSES.....	17
3.2 LAWS GOVERNING HEAT AND MASS DIFFUSION.....	18
3.3 CONSERVATION.....	18
3.4 CONSERVATION EQUATIONS.....	19
3.5 INTEGRAL AVERAGING BY VOLUME.....	21

3.6 REACTION KINETICS .....	23
3.7 A GENERAL MODEL.....	26
4. CONSIDERATIONS FOR THE MODELLING AND SIMULATION ENVIRONMENT .....	29
4.1 INTRODUCTION .....	29
4.2 PROBLEM SOLVING ENVIRONMENTS.....	30
4.3 TYPICAL SIMULATION NEEDS .....	31
4.4 GEST SPECIFICATIONS.....	32
4.5 QUALITY CRITERIA FOR MODELLING AND SIMULATION INTERFACES.....	35
4.5.1 <i>Some Interface Requirements for GestCell</i> .....	36
4.5.2 <i>Convenience Criteria - GestCell</i> .....	37
4.5.3 <i>Reliability Criteria - GestCell</i> .....	38
4.5.4 <i>Adjustability Criteria - GestCell</i> .....	38
5. ARCHITECTURE AND FUNCTIONALITY OF GESTCELL .....	40
5.1 ARCHITECTURE OF GESTCELL .....	40
5.1.1 <i>Procedures for Processing the Gest Specification</i> .....	42
5.1.2 <i>Pointers to information in Gest Specifications</i> .....	42
5.2 USING GESTCELL.....	43
5.2.1 <i>Editing Gest Specifications</i> .....	47
5.2.2 <i>Specifying Parameter and Initial Value Sets</i> .....	49
5.2.3 <i>Editing Experiment Specifications</i> .....	51
5.2.4 <i>Generating the Executable File for Simulation Runs</i> .....	53
5.2.5 <i>Performing Simulation Runs</i> .....	54
5.2.6 <i>Retrieving and Analysing Output Data</i> .....	56
5.3 A GEST SPECIFICATION CONSTRUCTED USING GESTCELL.....	56
5.4 SIMULATION OF THE PEMFC USING GESTCELL .....	59
6. CONCLUSIONS AND FUTURE WORK .....	62
6.1 ACHIEVEMENTS .....	62
6.2 FUTURE WORK .....	63
REFERENCES .....	64
APPENDICES: AN EXAMPLE PROBLEM.....	67
APPENDIX A: PEMFC MODEL AND SIMULATION IN GESTCELL .....	68
APPENDIX B: PEMFC MODEL AND SIMULATION IN ACSL .....	75

## **1. Introduction**

The work presented in the following pages represents the development of a modelling and simulation tool to be used for studying the Proton Exchange Membrane Fuel Cell (PEMFC). The development of this software required a multidisciplinary approach, or a systems approach, to develop a simulation tool that allows the user to formulate and modify models in order to simulate a Proton Exchange Membrane Fuel Cell (PEMFC).

### **1.1 Motivation**

The proton exchange membrane fuel cell (PEMFC) is a technology that has a number of characteristics which make it attractive for further development. The application areas of this technology include space applications, where it has already been used, electric vehicles and military applications. Some of the attractive features include: clean energy conversion, availability of construction materials, a solid electrolyte (no danger of leakage of harmful chemicals), low temperature operation, ease of stacking, and tolerance to CO<sub>2</sub>.

A number of steady state models of the PEMFC have been proposed in an attempt to better understand the functioning of the cell and improve its performance. Some steady state models have been successful in reproducing observed performance of the PEMFC. However, these models usually include one or more parameters for which there is not a known value. The unknown value(s) is usually adjusted to produce a good fit with the data. Therefore past models are somewhat limited in predictive ability. However, these steady state models have been very useful in gaining insight in how to improve the design and operation of the PEMFC.

There are a number of physical and electrochemical processes occurring within the PEMFC. For the most part these processes are fairly well understood. However, when these processes interact in various ways within the PEMFC, this real world system becomes extremely complex. In principal, it should be possible to develop dynamic models that can describe the performance of

the PEMFC, based on the theoretical knowledge of the processes within the PEMFC. Indeed, the steady state models that have been proposed in the past contain a great many insights that could be used in the development of such models. Such models would be complex and would be analysed most easily with simulation studies rather than solving for analytical solutions.

There are a number of technical problems that must be investigated in order to ensure that the PEMFC will become practical for future use. Water transport within the electrolyte membrane is a particularly important problem that has received attention in the electrochemical literature. Achievability of high current densities, while maintaining high efficiency operation, is the primary goal in order to make this technology viable. Other areas that could be investigated are: maximization of fuel cell efficiency, maximization of PEMFC service life, cost effectiveness of design (e.g. excess catalyst (platinum) loading significantly raises the cost of construction). These areas and many more could be studied using dynamic models and simulation in order to improve the design and operation of the PEMFC.

## **1.2 Structure of the Thesis**

The goal of this thesis is to develop a modelling and simulation environment that will allow the user to formulate dynamic models of the PEMFC, as well as modify these models and perform simulation runs/studies. The environment GestCell implements the Gest language developed by Ören (1984).

The first portion of the thesis is devoted to outlining the problem from the point of view of the real world system, the Proton Exchange Membrane Fuel Cell (PEMFC). A general description of the technology and function will be presented. A general discussion of the issues related to dynamic modelling for the system is presented, and provides a fairly complete outline of the features any particular dynamic model might include.

Chapters 2 and 3 present the fuel cell material. A general discussion of fuel cells is followed by a survey of the modelling and simulation that has been done with respect to the Proton Exchange Fuel Cell (PEMFC) in particular. Issues related to dynamic modelling of PEMFCs are given consideration in Chapter 3 and summarized.

In chapter 4, the requirements for a modelling and simulation environment are discussed, both in general and with respect to the particular problem area of the thesis. Following the analysis of the user needs for modelling and simulation, chapter 5 presents the particular approach undertaken in the development of the GestCell system. Both the functionality and the architecture of the modelling and simulation system are outlined. The appendices contain an example of an application of GestCell in the development of a dynamic PEMFC model..

## 2. Fuel Cells

A fuel cell is an energy conversion device, which converts the chemical energy of a fuel and oxidant, often hydrogen and oxygen, to electrical energy. Fuel cells are similar to batteries, however, unlike a battery a fuel cell must be continuously provided with fuel, rather than deriving energy from materials contained within the cell, and the products of the electrochemical reaction must be removed from the cell. A fuel cell will continue to provide electricity as long as fuel is supplied to the cell (Fickett, 1984). The fuel cell has become a good candidate for an alternative type of energy conversion device for a number of reasons. Some of these include: the need for energy sources that do not contribute to environmental problems associated with emissions from fossil fuel burning, the depletion of fossil fuel reserves, the attractiveness of low noise from plants, the high potential for fuel efficiency, and the development of new materials since initial demonstrations as long ago as 1839 (Fry, 1993).

Fuel cell systems are a promising technology, that has the potential to offer low-noise, low-emission and high-efficiency energy conversion in the not too distant future (Kordesch & Oliveira, 1985). The fundamental processes in fuel cells are fairly well understood, and are quite similar to batteries. However, in theory and practice fuel cells and fuel cell systems can become quite complex, making it impossible to fully understand their functioning analytically. Therefore, simulation is a necessary tool to develop this technology further.

### 2.1 General Description of a Fuel Cell

The three major components of the fuel cell are the anode, the cathode and the electrolyte:

- The *anode* is the electrode at which the fuel oxidation takes place.
- The *cathode* is the electrode at which the oxidant reduction reaction takes place.
- The *electrolyte* provides a medium for the transport of one of the ionic species involved in the electrochemical reactions in the fuel cell.

In a fuel cell, the fuel and oxidant are usually provided in gaseous form at the electrodes, which are normally porous. The electrodes serve as an interface between the reactants and the electrolyte, in order that the electrochemical reactions may occur. The electrolyte also serves the purpose of separating the gaseous reactants, allowing only the transport of the necessary ions for the energy conversion (Anahara, et al., 1993).

The electrodes of the fuel cell usually require the presence of a catalyst (e.g. platinum), which introduces problems such as deterioration of the catalyst. In addition to the cell itself, a fuel cell system must also have some accessories that provide the cell with the fuel and oxidant, as well as removing the product(s) of the electrochemical reactions. Different types of fuel cells will only function in certain temperature ranges. The reactions in a fuel cell are exothermic, so there is heat produced by the cell as well as electricity, often requiring some type of cooling. These factors and others serve to make fuel cell systems potentially very complex.

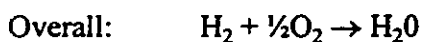
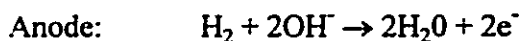
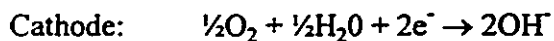
## **2.2 Types of Fuel Cells**

It is practical to classify fuel cells in terms of their electrolytes. The five most common types of fuel cells are: The Alkaline Fuel Cell (AFC), the Phosphoric Acid Fuel Cell (PAFC), the Molten Carbonate Fuel Cell (MCFC), the Solid Oxide Fuel Cell (SOFC), and the Proton Exchange Membrane Fuel Cell (PEMFC).

### **2.2.1 The Alkaline Fuel Cell (AFC)**

The AFC has an aqueous solution of potassium hydroxide as an electrolyte. Low-cost carbon and plastics can be used in the construction of the cell and electrodes. A number of catalysts are available, contrary to acidic cells. These fuel cell systems yield the highest voltage of all fuel cell systems at comparable current densities (Kordesch & Oliveira, 1985).

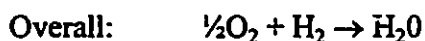
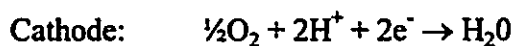
Reactions:



### 2.2.2 The Phosphoric Acid Fuel Cell (PAFC)

As the name implies, the electrolyte in the PAFC is a solution of highly-concentrated Phosphoric acid. The electrodes are made of carbon with a noble metal catalyst (e.g. platinum). The main advantage of the PAFC is that it rejects  $\text{CO}_2$ , which may be present in the reactant gases, when produced from fossil fuels (Kordesch & Oliveira, 1985).

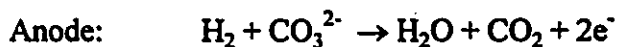
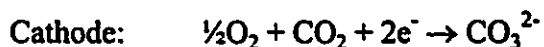
Reactions:



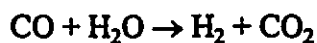
### 2.2.3 The Molten Carbonate Fuel Cell (MCFC)

The electrolyte in this cell is carbonate (e.g. lithium, sodium, and/or potassium carbonates). At present, the electrodes are made of nickel, treated with oxides (anode), and lithiated sintered nickel oxides (cathode). The MCFC is a high temperature fuel cell. The main problem is availability of materials that can withstand the severe operating conditions, all of which are presently costly (Kordesch & Oliveira, 1985). One example of reactions used to describe this fuel cell are presented below, although the reaction at the cathode is not yet well understood (Kordesch & Oliveira, 1985, p. 74).

Reactions:



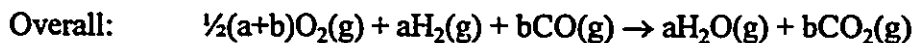
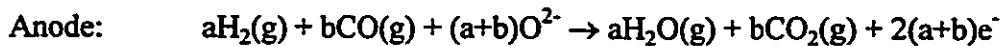
Shift Reaction: (occurs in the presence of CO)



### 2.2.4 The Solid Oxide Fuel Cell (SOFC)

A solid mixture of yttria ( $Y_2O_3$ ) and zirconia ( $ZrO_2$ ) is used as the electrolyte. Examples of electrodes that have been used are nickel/zirconium oxide cermet (anode) and lanthanum manganate ( $LaMnO_3$ ). This is the highest temperature fuel cell (Kordesch & Oliveira, 1985).

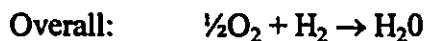
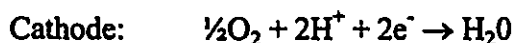
Reactions:



### 2.2.5 The Proton Exchange Membrane Fuel Cell (PEMFC)

Usually, the PEMFC uses a proton exchange membrane as an electrolyte, hence its name, the proton exchange membrane fuel cell (PEMFC). Nafion<sup>®</sup>, a sulfonated polytetrafluoroethylene, manufactured by DuPont, a membrane manufactured by Dow, and Aciplex-5 (Asalie) are examples of membranes that have been used. It is necessary to humidify the gas fed to the PEMFC. Electrodes are made of carbon with a Platinum catalyst and are pressed onto the membrane. Water transport, through the electrolyte, which must be hydrated, is one of the main problems associated with the PEMFC (Kordesch & Oliveira, 1985).

Reactions:



In the PEMFC, this chemical reaction will theoretically correspond to a potential difference of 1.229 V.

**Table 1. Types of Fuel Cells**

Type	Electrolyte	Temperature (°C)	Issues	Likely Applications
AFC	aqueous KOH solution	60-120	CO <sub>2</sub> troubles	electric vehicles, space, military
PAFC	concentrated Phosphoric Acid	160-220	CO sensitivity of the electrodes	cogeneration systems (~160°C)
MCFC	mixture of molten carbonates (Li <sub>2</sub> CO <sub>3</sub> /K <sub>2</sub> CO <sub>3</sub> )	600-650	CO <sub>2</sub> - makes recycling of electrolyte necessary	dispersed and/or cogeneration systems (~600°C)
SOFC	Ceramic ZrO <sub>2</sub> , Y <sub>2</sub> O <sub>3</sub>	800-1000	ceramic cells	dispersed and/or cogeneration systems (~1000°C)
PEMFC	polymer membrane	60-120	humidification of reactant pores	electric vehicles, space, military

The problem of this thesis is to develop a simulation environment for the last type of fuel cell, the PEMFC. As such, any further discussion of fuel cells will refer to PEMFC.

### **2.3 Energy Losses Within the Cell**

The performance of a fuel cell is measured as a relationship between current and voltage. Energy losses within the cell reduce cell voltage at higher currents. Fuel cells are an efficient energy conversion device, however, there are a number of factors that cause energy losses, resulting in decreased voltage output. An important example is the performance of the PEMFC is effected by the amount of water contained in the polymer electrolyte. At the anode the electrolyte can become dehydrated, while the region around the electrolyte/cathode interface may become flooded by the production of water. (Kordesch & Oliveira, 1985). Hence, water management is an important issue in trying to obtain good performance from the PEMFC.

Generally, the performance of a fuel cell will improve at higher temperatures and higher pressure (but the lifetime of the cell will decrease). However, there are a number of energy losses within a fuel cell that must be taken into account when discussing fuel cell performance.

### 2.3.1 Activation polarization

Activation polarization refers to the initial energy required to allow the electrochemical reactions at the electrodes, to proceed. In general, the activation energy lost is described by the equation (Fickett, 1984):

$$pol_{act} = a + b \ln i$$

where:  $pol_{act}$  = activation polarization, mV

$a, b$  = constants

$i$  = current density, mA/cm<sup>2</sup>

The activation polarization can be calculated for each electrode independently and added to give the activation polarization for the cell:

$$pol_{act(cell)} = pol_{act(anode)} + pol_{act(cathode)}$$

### 2.3.2 Ohmic polarization

This refers to the drop in voltage due to ohmic losses or resistance within the cell. There may be electronic impedance at the electrodes or any contacts within the cell, as well as ionic impedance through the electrolyte. All of these losses follow Ohm's Law (Fickett, 1984):

$$pol_{ohm} = iR$$

where:  $pol_{ohm}$  = ohmic polarization, mV

$i$  = current density, mA/cm<sup>2</sup>

$R$  = total cell impedance, Y·cm<sup>2</sup>

### 2.3.3 Concentration polarization

This refers to the energy lost due to mass transport effects. For example, reactants must diffuse to and products must diffuse away from reaction sites, and there is a limit to how quickly the diffusion processes may proceed. This limit is reached at the limiting current density. The concentration polarization is described by the equation (Fickett, 1984):

$$pol_{conc} = (RT/nF)\ln(1 - (i/i_L))$$

where:  $pol_{conc}$  = concentration polarization, mV

$T$  = temperature, K

$n$  = number of electrons

$F$  = Faraday's constant (96,487 C)

$i$  = current density, mA/cm<sup>2</sup>

$i_L$  = limiting current density, mA/cm<sup>2</sup>

The concentration polarization can be calculated for each electrode independently and added to give the activation polarization for the cell:

$$pol_{conc(cell)} = pol_{conc(anode)} + pol_{conc(cathode)}$$

The expressions for the different types of polarization in a fuel cell describe Figure 1, a possible polarization curve for a PEMFC.

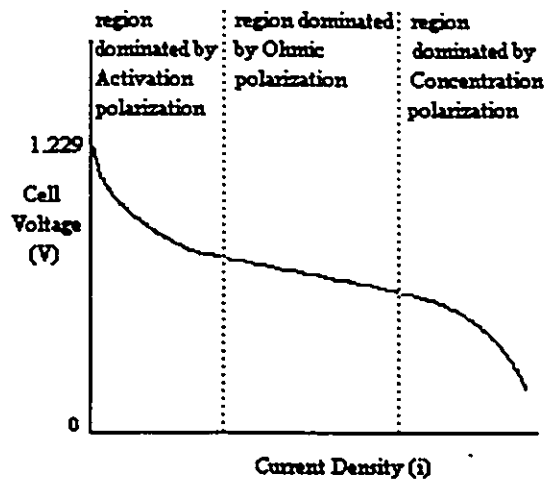


Figure 1. Possible Polarization curve for a PEMFC

## 2.4 Survey of Mathematical Models of the PEMFC

Fuel cells can be modelled at a number of levels. There are several processes and subsystems occurring within a fuel cell as discussed earlier. Electrode processes, membrane (electrolyte) properties, individual fuel cells, fuel cell systems, etc. can all be modelled at various levels of abstraction and complexity. A number of models for single cells have been proposed. Some of these models are presented below.

### 2.4.1 Springer, et. al.

Springer, Zawodzinski & Gottesfeld (1991) presented a model of a single cell polymer electrolyte fuel cell, in order to consider resistive losses due to partial dehydration of the electrolyte, as well as cathode flooding problems which result from the presence of too much water in the cell. Water management is an important aspect of the PEMFC, because water within the membrane is transported through diffusion as well as electro-osmotic drag. Water is produced at the cathode as well as fed to the cell in the cathode feedstream. Hydration of the

membrane is necessary for operation but excess water at the cathode will decrease cell performance.

Specifically, the model calculated water flow through five regions in the cell, from the anode to the cathode. Thus, the differential equations in the model are taken with respect to the distance from the anode in the direction of the cathode (i.e.,  $z$ ) rather than with time as the independent variable. The model assumes an isotherm for water sorption into the membrane, which has been determined experimentally. Therefore, one can refer to this model as an isothermal, one-dimensional ( $z$ ) model of a fuel cell. The majority of the parameters used in the model were experimentally derived, in order to make the model as valid as possible.

The authors computed a solution to the system of equations by integrating with respect to  $z$ . They found the simulation results possessed two major discrepancies with experimental data. First, the model did not predict a need to humidify the cathode stream, when, in practice, it is necessary to do so to achieve adequate performance. The authors suggested this was a result of not including evaporative losses of water in the cathode gas stream, in the model. Second, the model did not consider the effect of excess liquid water at the cathode, which would effect protonic conductivity, and act as a barrier for reactant gas (Springer. et al., 1991).

Nonetheless, when the fuel cell was operated under conditions with no excess liquid water at the cathode, this model was close to experimental data.

Springer, Wilson & Gottesfeld (1993) presented a further modelling effort meant to highlight performance limitations to the PEMFC found in the cathode of the fuel cell. This paper produced a good fit between model results and experimentally observed data. Importantly, the paper presents complete polarization curves for the PEMFC model, whereas earlier models were not as successful at producing the limiting current density portion of the polarization curves.

Another interesting feature of this model was the use of an effective oxygen concentration in the gas flow channel. This average value for oxygen concentration is in contrast to the alternative approach of modelling the concentration distribution along the gas flow channel. The authors point out that this effective value for oxygen concentration, a simple average between the inlet and outlet concentrations, is effective in modelling the processes in the cathode.

#### **2.4.2 Bernardi & Verbrugge**

Bernardi and Verbrugge (1992) subsequently presented a model of the PEMFC, with a number of features not modelled by Springer et al. Some of the more important differences included were: pressure-driven flow of water through cell components, a distinction between gas and liquid water, electronic resistance of the electrodes, and electrochemical reaction resistance at the anode. However, unlike the earlier model, this model did not allow for simulation with partial dehydration of the membrane.

Some of the basic assumptions in Bernardi and Verbrugge's model included: constant temperature(s), all gases were considered ideal and well mixed, the z direction proceeded from anode to cathode, the gas feed streams were at a higher temperature than the cell. All but two of the parameters in the model were determined from experimental data. The remaining two parameters were adjusted to improve the fit of the model.

Again, the simulation produced results close to experimental data, including a prediction that a newer membrane manufactured by Dow would result in higher cell performance than with the Nafion<sup>®</sup> membrane.

#### **2.4.3 Fuller & Newman**

Following these two one-dimensional models, Fuller and Newman (1993) presented a model in two dimensions, and including thermal effects on cell performance. These two features were included in addition to many of the features in the two previous models. The two dimensions

considered were  $y$ , similar to  $z$  in the previous two models, and,  $z$ , the distance along the length of the cell. The second dimension considered the position of the gas in the feed channel.

The main focus of this model was to consider water transport from anode to cathode, including water supplied and recycled water, dehydration of the anode, and flooding of the cathode. The model did not consider condensation of water among the effects of variable temperature.

Fuller and Newman (1993) concluded that thermal considerations were required in order to optimize the performance of PEMFCs. They mentioned that controlling the temperature, however, was difficult because the heat-transfer requirements varied with current density.

#### **2.4.4 Nguyen and White**

Finally Nguyen and White (1993) offered a two-dimensional, steady-state, heat and mass-transfer model of the PEMFC. The authors stated that this model was more applicable than the previous research, which was isothermal. They assert that this previous assumption makes the earlier models unsuitable for water and heat management studies.

The assumptions made by Nguyen and White (1993, p. 2179) are as follows:

- temperature of the solid is uniform and constant,
- flow of the gases is plug-flow,
- total pressure is held constant,
- heat transfer in the gas phase is negligible,
- water at the electrodes in the gas channels is vapour only,
- gas-diffusion through the electrode layer is neglected,
- the gas mixture is ideal,
- liquid water takes the form of small droplets, and the volume is negligible,
- the electro-osmotic coefficient, and the diffusion coefficient are determined by activity in the anode flow channel,

- there was no voltage drop along the flow channels.

The authors used their model to consider 2 alternative humidification designs, as well as humidification problems associated with air operation. First, as a base case they considered a conventional humidification design featuring water vapour and a gaseous reactant fed to the fuel cell. Secondly, they considered an alternative design featuring injection of liquid water into the feed stream.

The authors concluded that when operating at high power densities and energy efficiency, back diffusion of water from the cathode to the anode was insufficient to keep the membrane hydrated. Furthermore when air was used in the cathode feed stream, it was necessary to humidify the stream.

#### **2.4.5 RMC Model**

Amphlett et al. (1993) have formulated a parametric model of a PEMFC stack based data obtained using a Ballard Mark IV single cell. The form of the relationships between current, voltage, pressure and temperature are based on intuitive mechanistic principles about the functioning of the PEMFC. The model equations were fit to the data using linear regression.

The numerical values calculated for the parameters in the model made intuitive sense to the researchers. For example, increases in temperature and oxygen concentration reduce activation polarization, through positive effects on reaction rates.

The model showed a very good correlation with the experimental data used in its estimation. Based on the fact that the model was based on mechanistic principles and took into account interactions among the variables, the authors feel the predictive capability of the model is useful over a broad range of operating conditions, outside the operating conditions used to construct the model.

The most obvious use for such a model is to predict the performance of the Mark IV cell for a given set of operating conditions. Furthermore, the authors feel their model is useful in defining trends in fuel cell performance for systems integration considerations. The model does elucidate a number of factors in PEMFC operation. For instance, the authors point out that the model indicates that temperature changes have a more pronounced effect on voltage at higher currents than at lower currents. Undoubtedly, this type of model does help to better the understanding of fuel cell performance, and importantly demonstrate the complexity of a fuel cell system.

## **2.5 Summary of Steady State Models and Simulation**

A number of complex steady-state models have been used successfully to predict polarization curves of PEMFCs. Past research has not focussed on developing dynamic models for simulation of PEMFCs. It is fair to say that modelling and simulation efforts have made progress in understanding some aspects of PEMFCs, such as distribution of water in the electrolyte membrane. This has assisted the continuing development of steady-state models. This has undoubtedly led to a better understanding of the present designs for PEMFCs and their performance capabilities. (Keon, et al., 1995) Simulation of PEMFCs is progressing, such that reliable prediction of the performance of a hypothetical PEMFC over time and over a wide range of operating conditions seems to be achievable.

### **3. Dynamic Modelling of the PEMFC: Issues**

Contrary to the steady state models discussed above, it is possible to consider a dynamic model of the Proton Exchange Membrane Fuel Cell (PEMFC). A dynamic model of the PEMFC must consider at least two aspects of the fuel cell's operation, which are discussed below. Transport processes govern the movement of reactants and water fed to the cell with the reactant gases, reaction products (water), and any other gases within the PEMFC, as well as the transport of heat within the cell. Reaction kinetics describe the dynamics of the chemical reactions that occur within the PEMFC.

#### **3.1 Transport Phenomena Processes**

Transport phenomena processes are the processes by which mass, heat and momentum move within a system. The two main processes are known as diffusion and convection and apply to all three quantities mentioned above. An example of diffusion is the movement of a gas or liquid caused by a concentration gradient, or the transport of heat caused by a temperature difference across a region. Diffusion of mass and heat can cause movement of a gas or heat through a barrier. This type of diffusion can be seen in the Proton Exchange Membrane Fuel Cell (PEMFC), for instance as the gases and heat are transported through the electrodes. Convection is the type of transport process that occurs due to the bulk flow of material within a system. (Beek & Mutzall, 1975) Migration is a transport process effecting the movement of charged species, or ions, due to electrical forces caused by a potential gradient. This transport process is important in solutions of ionic electroactive species (Britz, 1981). In the case of the PEMFC, diffusion is more important than convection, and migration could likely be ignored, because of the inert electrolyte membrane.

### 3.2 Laws Governing Heat and Mass Diffusion

The fluxes of both mass and heat are proportional to the gradient that acts as the driving force for a particular type of transport. Fick's law in the case of mass transport, and Fourier's law in the case of heat transport are presented by Beek & Mutzall (1975, p. 12):

$$\bar{j} = -D \frac{dc}{dn} \quad \text{Fick's law}$$

where,

$$\bar{j} = \text{mass flux, kg/m}^2\text{s}$$

$$D = \text{mass diffusivity}$$

$$\frac{dc}{dn} = \text{concentration gradient}$$

$$\bar{q} = -a \frac{d(\rho c_p T)}{dn} \quad \text{Fourier's law}$$

where,

$$\bar{q} = \text{heat flux, W/m}^2$$

$$a = \frac{\lambda}{\rho c_p} = \text{thermal diffusivity}$$

$$\lambda = \text{heat conductivity}$$

$$\frac{d(\rho c_p T)}{dn} = \text{heat gradient}$$

### 3.3 Conservation

Beek & Mutzall (1981, p. 3) state the principle of conservation as follows. where X is a certain quantity.

$$\frac{\text{accumulation of X in system}}{\text{unit time}} = \frac{\text{flow of X into system}}{\text{unit time}} - \frac{\text{flow of X out of system}}{\text{unit time}} + \frac{\text{production of X in system}}{\text{unit time}}$$

Mass, heat and momentum in the PEMFC are all conservative quantities.

### 3.4 Conservation Equations

This sections below discuss the principle of conservation in the form of mathematical equations for conservation of mass and energy. For simulation purposes ordinary differential equations are much simpler to handle, and a basis for justifying the use of ordinary differential equations is presented in the section Integral Averaging by Volume.

In order to model transport phenomena processes in the PEMFC, it is necessary to discuss conservation equations. Stanislav (1982, pp.21-25) states the laws of conservation of mass and energy as follows:

**Conservation of Mass (Continuity Equation):**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{v}) = 0$$

where,

$\rho$  = mass density, M/L<sup>3</sup>

$\nabla$  is a gradient

**For a multicomponent system:**

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\bar{j}_i + \rho_i \bar{v}) = R_i$$

where,

$\rho_i$  = mass density of species  $i$ ,  $M/L^3$

$\vec{j}_i$  = diffusional flux of species  $i$ ,  $M/tL^2$

$\vec{v}$  = bulk flow of material,  $L/t$

$L$  = Length

$\nabla$  is a gradient

Note:  $\sum_{i=1}^N R_i = \sigma_M = 0$

$\sigma_M$  = rate of mass production

### Conservation of Energy (Energy Equation):

$$\sigma_E = 0$$

where,

$\sigma_E$  = rate of energy production

For a multicomponent system:

$$\rho \frac{D}{Dt} \left[ \hat{U} + \frac{1}{2} v^2 \right] + \nabla \cdot \left[ \vec{q} + \vec{v} \cdot \vec{p} \right] = \rho \hat{F} \cdot \vec{v}$$

where,

$\hat{U}$  = internal energy,  $ML^2 / t^2$

$\vec{q}$  = energy flux,  $M / t^3$

$\vec{p}$  = stress tensor,  $M / Lt^2$

$\hat{F}$  = force,  $ML / t^2$

$\rho, \vec{v}, \nabla$  same as above

The above equations are stated with respect to three space variables and time. Fortunately it is possible to simplify the equations a great deal and arrive at an ordinary differential form for the conservation laws which are central to modelling transport phenomena.

### 3.5 Integral Averaging by Volume

The above equations can be integrated over a small volume in order to yield equations expressed in terms of average values for mass and energy for a given volume. This has the desirable result of reducing the above partial differential equations in four dimensions to ordinary differential equations with respect to time. Stanislav (1982, pp. 18-19) presents two theorems which facilitate this simplification.

Gauss-Ostrogradskii Divergence Theorem:

$$\iiint_V \nabla \cdot \bar{a} dV = \iint_A (\bar{n} \cdot \bar{a}) dA$$

where,

$\bar{a}$  = a vector quantity

$\bar{n}$  = the outwardly directed unit normal vector

$V$  = a closed region in space surrounded by a surface  $A$

Reynolds Transport Theorem:

$$\frac{d}{dt} E = \iiint_{V(t)} \frac{\partial I}{\partial t} dV + \iint_{A(t)} I(\bar{v} \cdot \bar{n}) dA$$

where,

$$\frac{d}{dt} E = \iiint_{V(t)} \frac{\partial I}{\partial t} dV + \iint_{A(t)} I(\bar{v} \cdot \bar{n}) dA$$

$E(x, y, z, t)$  = an arbitrary scalar extensive quantity

$I(x, y, z, t)$  = the corresponding intensive quantity to  $E$

$V(t)$  = time variable volume

$A(t)$  = time variable surface

$\bar{v}$  = bulk flow rate

$\bar{n}$  = same as above

Using these two theorems and averaging the partial differential form of the conservation laws over a fixed volume it is possible to demonstrate the following ordinary differential forms of the conservation laws applied to transport phenomena processes. (Stanislav, 1982, pp. 56-63)

Continuity Equation:

$$\frac{d}{dt} m_i = -\mathfrak{I}_i$$

where,

$$m_i = \iiint_V \rho_i \, dv$$

$$\mathfrak{I}_i = \iint_A [\bar{j}_i + \rho_i \bar{v}] \, d\bar{A}$$

$m_i$  = mass of  $i$ th component

$\rho_i$  = density of  $i$ th component at point  $(x, y, z)$

$\mathfrak{I}_i$  = net efflux of  $i$ th component, including diffusional flux ( $\bar{j}_i$ )  
and convective flux ( $\rho_i \bar{v}$ )

Energy Equation:

$$\frac{d}{dt} E = -\Delta(w\hat{E}) + Q - W - \Delta(p\hat{V}w)$$

where,

$$\Delta(w\hat{E}) = - \iint \rho \hat{E} \bar{v} \cdot d\bar{A}$$

$$Q = \iint_{A_s} \bar{q} \cdot d\bar{A}$$

$$W = \iint_{A_w} \bar{v} \cdot \vec{P} \cdot d\bar{A}$$

$$\Delta(p\hat{V}w) = \iint_{A_1 + A_2} \bar{v} \cdot \left( \vec{pl} \right) \cdot d\bar{A}$$

$\Delta(w\hat{E})$  = net free rate of energy transfer by convection

$Q$  = net rate of heat added to the system by conduction across the solid surface

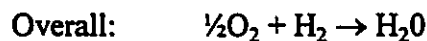
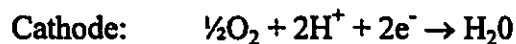
$W$  = work done by pressure and viscous forces of the system on the surroundings

$\Delta(p\hat{V}w)$  = the rate of work done by pressure forces needed to supply and remove the material to and from the system

When formulating a model it is possible to write the differential equations directly, based on the general law of conservation discussed above. However, if one is unfamiliar with the system in question the equations can be written and simplified in the manner presented in the previous two sections (Stanislav, 1982). Furthermore, the above sections should convince the reader that for a small volume, it is reasonable to use ordinary differential equations for quantities being considered in a dynamic model of the PEMFC.

### 3.6 Reaction Kinetics

In the case of the PEMFC, there are electrochemical reactions occurring at either electrode. Therefore, it is necessary to describe the behaviour of these reactions with respect to a number of parameters and time in order to model the rates at which the reactions will occur. The equations giving these rates of reaction are determined by the reaction kinetics. Recall the equations for the electrochemical reactions occurring at the electrode:



However, the reaction kinetics depend on the specific pathway of a reaction. In other words, the rate at which a reaction occurs depends on the specific way in which the overall reaction occurs, including intermediate steps. It is not necessarily true that the stoichiometric equation of a reaction (e.g. the three reactions stated above) are the same as the specific pathway by which the reaction occurs (Segal, 1985, p.734). In fact, in the case of the PEMFC, the stoichiometric

equations are not the specific pathway of the reaction, which should be clear because there is a catalyst involved in the electrode reactions. A suggested specific pathway for the PEMFC is presented below (Koene, F.G.H., et. al., 1993).

At the Anode:

1.  $H_2 \rightarrow HH^*$  (hydrogen molecule is excited)
2.  $HH^* \rightarrow H + H$  (dissociation into 2 H atoms)
3.  $2(H \rightarrow H^+ + e^-)$  (dissociation into protons and electrons)

At the Cathode:

1.  $O_2 + e^- + H^+ + e^- + H^+ \rightarrow HOOH$  (absorption of an electron, a proton, and another electron and proton)
2.  $HOOH \rightarrow HOOH^*$  (peroxide excited)
3.  $HOOH^* \rightarrow HO + HO$  (dissociation into two hydroxides - the rate determining step; energy barrier  $\sim 2.2\text{eV}$ )
4.  $(OH + e^- + H^+) \rightarrow 2H_2O$  (each OH absorbs an electron and a proton)

The reaction rate laws for the electrode reactions are determined by the "rate determining step," that is the slowest step in the process by which the reaction occurs (Segal, 1985, p. 734).

Therefore, the rate law for the reaction at the cathode is given by

$$\text{rate for the cathode reaction} = k^* [HOOH^*]$$

where,

$$\text{rate for the cathode reaction} = k^* [HOOH^*]$$

$k^*$  = rate constant for the reaction (third step at the cathode)

$[HOOH^*]$  = concentration of  $HOOH^*$  molecules at the reaction site

However, the rate should be expressed in terms of the original chemical species, not intermediate species such as  $\text{HOOH}^*$ . The relationship between intermediate species in one step and a species in another step are expressed by an equilibrium constant,  $K$ . The original rate expression can be manipulated using equilibrium constants to obtain the overall rate law in terms of the species in the overall reactions.

$$\text{rate for the cathode reaction} = k[\text{O}_2][\text{H}^+]^2$$

where,

$$\text{rate for the cathode reaction} = k[\text{O}_2][\text{H}^+]^2$$

where  $k$  = rate constant for the overall reaction

$[\text{O}_2]$  = concentration of  $\text{O}_2$  molecules at the reaction site

$[\text{H}^+]$  = concentration of protons ( $\text{H}^+$ ) at the reaction site

The cathode reaction determines the overall rate of the fuel cell. However, a similar expression could be derived for the reaction at the anode.

The rate constant,  $k$ , in the above rate equation is dependent on temperature. The dependence of the rate constant on temperature is given by the Arrhenius Equation stated below (Segal, 1985, p.729).

$$k = Ae^{-E_{act}/RT}$$

where,

$A$  = the frequency factor

$E_{act}$  = activation energy

$R$  = Ideal Gas constant

$T$  = temperature

### 3.7 A General Model

A very general model of the Proton Exchange Membrane Fuel Cell (PEMFC) will be considered in order to ensure that the development of a simulation tool will allow for many different PEMFC models to be formulated. In the figure below, most of the important processes occurring within the PEMFC are included. However, in any particular model it would not be necessary to include all of these processes, and it may be desirable to include things that are not included in the figure. However, the diagram should give the reader a good idea of how a PEMFC works and the dynamic processes and interactions that must be taken into account.

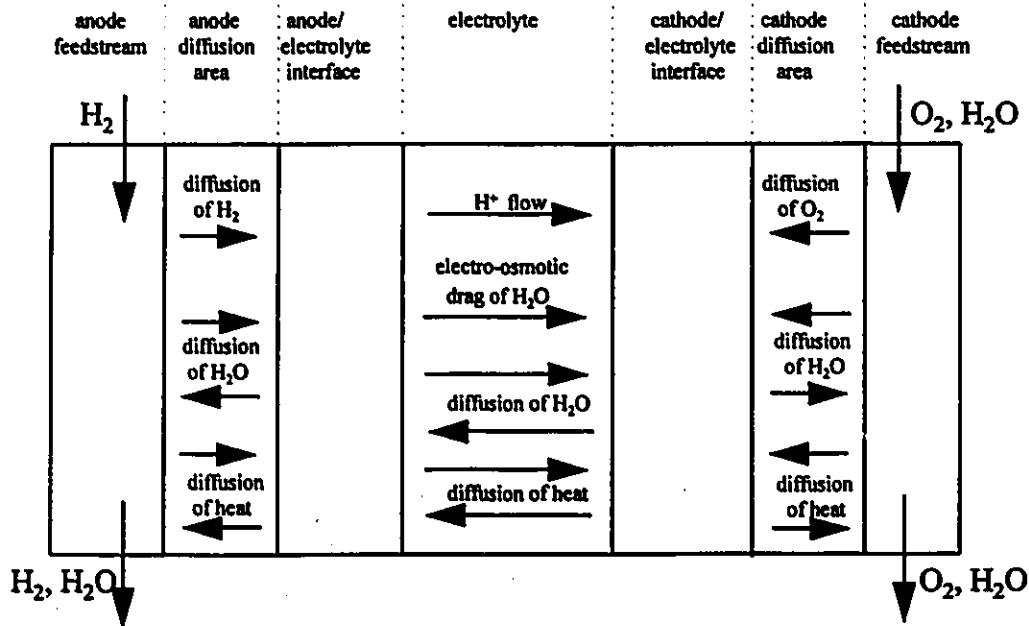


Figure 2. Diagram of the dynamic processes occurring within the PEMFC

Accompanying the diagram above, the following table lists many of the quantities and processes we might choose to include in a dynamic model of the PEMFC. In a model, one might prefer for certain quantities to state variables or parameters, depending on the emphasis of the model. Therefore the first row of the table refers to quantities that could either vary or be taken as parameters.

**Table 2: Components of Dynamic Model of the Proton Exchange Membrane Fuel Cell (PEMFC)**

	Anode Gas Channel	Anode	Electrolyte	Cathode	Cathode Gas Channel
<b>Quantities (State Variables and/or Parameters)</b>	<ul style="list-style-type: none"> <li>• mols H<sub>2</sub></li> <li>• mols H<sub>2</sub>O</li> <li>• Pressure</li> <li>• Temperature</li> </ul>	<ul style="list-style-type: none"> <li>• mols H<sub>2</sub></li> <li>• mols H<sub>2</sub>O</li> <li>• mols H<sup>+</sup></li> <li>• Potential difference</li> <li>• Pressure</li> <li>• Temperature</li> <li>• Current</li> </ul>	<ul style="list-style-type: none"> <li>• mols H<sub>2</sub>O (position within the electrolyte is important)</li> <li>• mols H<sup>+</sup> (position within the electrolyte is important)</li> <li>• Conductivity (resistance)</li> <li>• Pressure</li> <li>• Temperature</li> </ul>	<ul style="list-style-type: none"> <li>• mols O<sub>2</sub></li> <li>• mols H<sub>2</sub>O</li> <li>• mols H<sup>+</sup></li> <li>• Potential difference</li> <li>• Pressure</li> <li>• Temperature</li> <li>• Current</li> </ul>	<ul style="list-style-type: none"> <li>• mols O<sub>2</sub></li> <li>• mols H<sub>2</sub>O</li> <li>• Pressure</li> <li>• Temperature</li> </ul>
<b>Processes within Region</b>	<ul style="list-style-type: none"> <li>• Heat transport</li> </ul>	<ul style="list-style-type: none"> <li>• Diffusion of H<sub>2</sub> &amp; H<sub>2</sub>O</li> <li>• Heat Transport</li> <li>• Chemical Reaction (H<sub>2</sub> → 2H<sup>+</sup> + 2e<sup>-</sup>)</li> </ul>	<ul style="list-style-type: none"> <li>• Electro-osmotic Drag</li> <li>• Diffusion of H<sub>2</sub>O</li> <li>• Movement of H<sup>+</sup> across electrolyte</li> <li>• Heat Transport</li> </ul>	<ul style="list-style-type: none"> <li>• Diffusion of O<sub>2</sub> and H<sub>2</sub>O</li> <li>• Heat Transport</li> <li>• Chemical Reaction (O<sub>2</sub> + 4H<sup>+</sup> + 4e<sup>-</sup> → 2H<sub>2</sub>O)</li> </ul>	<ul style="list-style-type: none"> <li>• Heat Transport</li> </ul>
<b>Processes at Interface(s)</b>	<ul style="list-style-type: none"> <li>• Surface Diffusion of H<sub>2</sub></li> <li>• Surface Diffusion of H<sub>2</sub>O</li> <li>• Heat Transport</li> </ul>	<ul style="list-style-type: none"> <li>• Surface Diffusion of H<sub>2</sub> (Anode/Gas Channel)</li> <li>• Surface Diffusion of H<sub>2</sub>O (both sides)</li> <li>• Heat Transport</li> </ul>	<ul style="list-style-type: none"> <li>• Surface Diffusion of H<sub>2</sub>O (both sides)</li> <li>• Surface Diffusion of H<sup>+</sup> (both sides)</li> <li>• Heat Transport</li> </ul>	<ul style="list-style-type: none"> <li>• Surface Diffusion of O<sub>2</sub> (Cathode/Gas Channel)</li> <li>• Surface Diffusion of H<sub>2</sub>O (both sides)</li> <li>• Heat Transport</li> </ul>	<ul style="list-style-type: none"> <li>• Surface Diffusion of O<sub>2</sub></li> <li>• Surface Diffusion of H<sub>2</sub>O</li> <li>• Heat Transport</li> </ul>

## **4. Considerations for the Modelling and Simulation Environment**

### **4.1 Introduction**

In order to offer an effective tool for developing mathematical models and conducting simulation, it is necessary to understand the purpose of simulation. Ören (1994) offers a definition of simulation from a number of perspectives: technical, knowledge representation and processing, and pragmatic points of view. In a technical sense, simulation is “experimentation with dynamic models,” which includes the possibility of any number of types of dynamic models. From the point of view of knowledge representation and processing, simulation can be referred to as a “model based experiential knowledge generation activity.” Finally in the most pragmatic sense, “simulation offers the only logical choice to perform experimentations,” in cases where the real system is not available for some analysis or control problem.

All these views of simulation refer to a model. It is obvious to state that a model is necessary to conduct simulation. With good models, simulation allows us to generate worthwhile knowledge. Furthermore, a model that is not only accurate but can be easily modified will allow for much more general results to be generated using simulation. Any tool that assists in the development of accurate and reliable models, and allows flexibility in using models must serve to improve simulation. Therefore, it is reasonable to assert that an effective modelling tool, though not sufficient, is a necessary feature for a powerful simulation environment.

The previous chapters have discussed the overall problem area for which it is intended to offer a mathematical modelling and simulation environment. This environment must offer an effective way to develop models for the types of systems discussed earlier and permit simulation, as it is defined above, to be carried out. The current chapter focuses on the modelling and simulation needs that must be included in the proposed tool.

At this time it seems timely to introduce the system that is being developed for this thesis. The reasons for the name will become clear in the current chapter. In order to facilitate modelling and simulation of PEMFCs a tool named, "GestCell" has been developed.

## **4.2 Problem Solving Environments**

"A Problem solving environment is a computer system that provides all the computational facilities necessary to solve a target class of problems" (Gallopoulos, Houstis & Rice, 1994). Ideally a problem solving environment (PSE) should be able to solve problems over a range of complexity, offer opportunities for prototyping and/or analysis and be useful for purposes ranging from education to advanced research in a problem area. This may seem overly ambitious and may not be possible in all cases, but nonetheless, one should be aware that PSE's should be developed for the variety of needs, covering a wide range of potential users that exist for any problem area.

One reason that the development of effective PSEs is difficult and not often realized is the division between traditional areas of science and engineering. Highly trained engineers rarely have time to become proficient in areas of computation. Similarly computer scientists are rarely knowledgeable enough in other areas to develop PSEs single-handedly (Gallopoulos, Houstis & Rice, 1994). The development of an effective PSE for an engineering or science problem, requires knowledge from computer science as well as other areas of engineering and science. For example, to develop a simulation environment for PEMFCs requires knowledge from computer science, as well as chemistry, physics and mathematics. Several disciplines are required to develop a PSE, and the resulting tool should make knowledge from all the disciplines involved available to the user.

Gallopoulos, Houstis & Rice offer two generally accepted goals for PSE's: "they should enable more people to solve more problems more rapidly, and they should enable people to do things that they could not otherwise do" (Gallopoulos, Houstis & Rice, 1994). As has been shown from

the earlier survey of modelling and simulation activities, simulation is useful and necessary for the development of PEMFCs. However, as can be inferred from the relatively small amount of literature on the topic, simulation is not widely available to the scientists in this field. One factor that contributes to this situation is the fact that scientists who are knowledgeable in the area of PEMFCs are, quite understandably, not trained in the areas of simulation or computer science. Therefore, the development of an appropriate PSE for the simulation of PEMFCs will strongly meet the goals of PSEs as set out in the quotation above.

The notion of a problem solving environment offers a general idea of what makes a software tool both friendly and useful. A PSE is the type of tool that it is proposed to develop for the modelling and simulation of PEMFCs. Furthermore, it is likely that GestCell will be useful for solving other types of problems that share some of the features of models of PEMFCs.

### **4.3 Typical Simulation Needs**

Some or all of the following steps are typically carried out in order to solve a problem:

1. Construct a mathematical model of the phenomenon under study.
2. Select relevant physics and geometry.
3. Process equations and associated conditions, simplifying to allow suitable solution methods to be applied.
4. Specify a solution method based on analytical and approximate techniques.
5. Construct test problems and data sets.
6. Using an appropriate specification language, create or modify a specification of the problem.
7. Generate a corresponding program.
8. Apply the program to the test data.
9. Validate results.
10. Compare the quality of results and performance with alternative solution procedures.
11. Collect and manipulate output data.
12. Record the steps of the experiment.

13. Communicate the results to the scientific community.

(Gallopoulos, Houstis & Rice, 1994)

This is obviously a complex and time consuming activity and the development of a tool that allows some of these steps to be carried out more quickly or done automatically (e.g. programming in a traditional language such as C) increases the usefulness and availability of simulation to the user. It is suggested that in order to be useful to scientists in the study of PEMFCs, a simulation environment should make the construction and manipulation of mathematical models of the appropriate systems (PEMFCs) as friendly as possible, while making the actual simulation of the systems (ie. programming, numerical methods, and terminology specific to the field of simulation) as transparent to the user as possible. That is, the scientist should be able to perform a variety of activities with a mathematical model, using the knowledge he or she possesses about the system being studied, but should not be required to learn a great deal of new knowledge about simulation to do so.

#### **4.4 Gest Specifications**

In order to construct an environment for solving a class of simulation problems, one must consider how particular simulation problems will be defined. Traditionally the problem definition of mathematical models and experimentation is essentially two separate problems. The real world problem must be defined as a mathematical model, and the simulation run(s) to be carried out for that model, or the simulation problem(s) must be defined or programmed for the computer. As shall be explained below, Gest is a modelling and simulation language that simplifies the problem of defining a mathematical model and a simulation experiment (Ören, 1984). The Gest language will be used as the basis for a modelling and simulation environment, for the reasons outlined below.

Gest is a simulation language that is based on general system theoretic concepts, developed by Wymore (1967). Within Gest specifications of mathematical models and simulation experiments

are separated into sections. Gest is a specification language, which is sufficiently descriptive to serve the purpose of documentation of a mathematical model and/or simulation experiments. Gest is easily understandable, especially by individuals with little or no knowledge of programming languages. This is different from traditional languages, which can be difficult to understand without some knowledge of their syntax and structure. In this sense, Gest is different because it is intended at its foundation to present understandable models of systems for simulation experiments.

A Gest specification is also a systematic representation that functions as a programming language to run simulation experiments. Therefore a Gest specification of a model and experiment acts as both documentation and the programming code for simulation programs (Ören, 1984). This makes Gest very powerful in that it is understood by both the user and the computer. There are many benefits to this aspect of Gest, not the least of which are reducing the work required to produce a well-documented simulation study, and making simulation more available to users without an extensive background in computational science. The latter is true because there is a minimal need for learning a new language or methodology to conduct simulation, given the understandable nature of the specification.

In its original conception, a Gest program has three separate parts: a mathematical model, experiment specification(s) and output module(s) (Ören, 1984). The mathematical model presents the model in two parts: the declaration of the model elements and the specification of the dynamics of the model. The specification of the experiments provides the information related to the conditions under which the experiment will be conducted, such as parameter values, initial conditions and ending time, numerical methods, and error tolerances. The final module provides the instructions for output information. An outline of a Gest program is presented below, demonstrating the structure of a continuous model and the experiment specification.

```

Specification in GEST: Model, parameter set(s), initial value set(s) and experiment(s)

Continuous Model      Title
Model declarations
  Input variables
  State variables
  Output variables
  Auxiliary variables
  Constants
  Parameters
  Auxiliary parameters
  Tabular functions
Dynamic
  Input variables
  Auxiliary variables
  Derivatives
  Output functions
End model

Parameter set 1      Description
Parameters          values are specified
End parameter set 1

Initial Value Set 1  Description
State variables     initial values are specified
End Initial Value Set 1

Experiment 1
Observe
  Input variables
  Output variables
  State variables
  Auxiliary variables
Observe at every
  communication interval      eg. 0.25
Integrate by
  h          eg. Runge-Kutta 4
             integration step size      eg. 0.01
Start at
  tinit      initial time              eg. 0.0
Terminate when t >=
  tfinal     time condition            eg. 100.0
End experiment 1

```

**Figure 3. Outline of a Gest specification of a mathematical model and a simulation experiment**

In order to specify a simulation run in Gest, the user need only specify a parameter set, an initial value set and an experiment. The sets of values are associated with a particular model, so the system then has all the information necessary to perform a simulation run with only the three pieces of information mentioned above. Clearly, given a Gest specification, simulation is accessible, even to a non-programmer.

Because of its inherent strengths, Gest has been selected as the basis for GestCell, a mathematical modelling and simulation environment for the simulation of PEMFCs. The user

interface is intended to elicit from the user all the information necessary for constructing a complete Gest program in a transparent manner that requires very little knowledge of simulation methodology. The Gest specification is constructed in an intelligent manner by gathering from the user all the information in the mathematical model, without requiring the user to construct the specification manually. This prevents errors in the specification and allows the user to specify mathematical models in Gest without learning even this easily understood simulation language. Simulation runs are specified in the manner explained above, which requires very little learning on the part of the user.

#### **4.5 Quality Criteria for Modelling and Simulation Interfaces**

It is obvious that GestCell requires some kind of interface between the user and the simulation system. Indeed, a high quality interface is an area that offers a significant opportunity to make powerful simulation available to users because it makes the modelling and simulation environment friendly. The front-end interface of this tool must allow file-handling capabilities, the construction and editing of mathematical models of PEMFCs, the instructions to the system for carrying out the simulation experiments using the system. The back-end interface must allow the user to manipulate the data produced by the simulation experiments and produce useful and presentable output.

Ören & Ghasem-Aghaee (1995) have enumerated quality criteria for convenience, reliability and adjustability of user/system interfaces. Transparency, naturalness, simplicity, predictability, minimum memory load, consistency, navigability, productivity, informativeness, guidance, explanation, interpretation, and appeal are the quality criteria for convenience. Error prevention, error tolerance, and caution criteria are criteria concerning reliability. Adjustability criteria are adaptability, customizability, and maintainability. Ören & Ghasem-Aghaee (1995) also elaborate on the usefulness of the Visual Basic® programming language for developing graphical interfaces that meet these quality criteria.

Visual Basic® is used for developing the graphical interface for the modelling and simulation tool being discussed. The representation of Gest specifications in Excel are well-structured and easy to read. Microsoft Excel® is a spreadsheet package that comes equipped with a version of Visual Basic® called Visual Basic® for Applications®. The modelling and simulation environment being developed therefore is implemented in Excel® because of the nature of the Gest specification and the fact that Visual Basic® is readily available within Excel® for developing the interface. The functionality and architecture of the GestCell system will be elaborated upon in the next chapter.

#### **4.5.1 Some Interface Requirements for GestCell**

Because GestCell has been developed with a particular class of problems in mind, dynamic models of PEMFCs, certain considerations were taken into account while developing the modelling and simulation tool.

Steady state models of PEMFCs all share a number of features that are necessarily a part of future dynamic models as well. First of all, the models contain a large number of variables, parameters and constants. This makes for complex models that must be constructed systematically or confusion is inevitable. Furthermore, easy changes to parameter values are necessary in order to study a variety of scenarios. Gest is a suitable language for this type of problem because it requires the user to specify parameter values in sets. Similarly, the GestCell interface must allow the user to specify many parameter and initial value sets easily.

The dynamic models will not necessarily need a large number of state variables, however there are necessarily a large number of auxiliary variables and algebraic relationships. The interface of GestCell must make handling of large numbers of variables efficient and prevent errors from occurring due to the variety of variables. Auxiliary variables must be calculated in the correct order in computation in order to ensure that algebraic relationships are solved with the correct,

updated, values of variables. Therefore, it is necessary for GestCell to sort the auxiliary variables in the appropriate manner.

Another feature of simulation in PEMFCs is that the scientific community in this area has very little knowledge of simulation, as evidenced by the small volume of simulation work done in the area. Therefore, GestCell does not assume any knowledge of simulation on the part of the user. Therefore GestCell must allow the user to construct models based on scientific knowledge without requiring strict adherence to any particular language the user would have to learn.

#### **4.5.2 Convenience Criteria - GestCell**

Transparency is given emphasis in the current work. That is the very little training should be required for a user to develop mathematical models and perform simulation runs. (Ören and Ghassem-Aghaee, 1995). This is accomplished, in GestCell, through the use of dialog boxes that elicit all the information regarding a particular model element, parameter set, initial value set, experiment, simulation run(s) or output handling. All the interaction between the user and the system can be done through the dialog boxes which allows the user to simply input the knowledge about the system being modelled, and the software updates the Gest specification appropriately.

In Ören and GhassemAghaee's terminology naturalness refers to the fact that an interface is based on the user's own language and paradigm. Thus, information should appear in a natural and logical order to the user. In GestCell naturalness and simplicity are achieved thanks to the readable nature of the Gest specifications as well as the design of the dialog boxes. The user has the opportunity to input a great deal of information as part of a model but unnecessary terms are omitted from the Gest specifications by hiding unused sections of the model template. Furthermore, the Gest specification allows descriptions to be stored for any element of a model, which eliminates the need for comments, as in other programming environments.

### **4.5.3 Reliability Criteria - GestCell**

Ören and Ghassem-Aghaee (1994) offer error prevention and caution as two reliability criteria in interface design. Error prevention is given emphasis in GestCell, for example, by allowing the user to select variables and have them automatically inserted into equations in order to prevent typographical errors. GestCell also does a limited number of checks of the model before building the files used to perform simulation. If the equations specifying the auxiliary variables are not specified in certain order, the calculations can not be done. The values of all variables on the right hand side of an equation must be known before calculation. Therefore GestCell performs a sorting procedure automatically (similar to other continuous system simulation systems). Excel's® abilities are used for sorting. However, algebraic loops are not treated. GestCell is also a cautious system. Deleting and editing commands are always confirmed and the user is warned when files are being written that may replace files the user wants. GestCell then proceeds after a confirmation from the user.

### **4.5.4 Adjustability Criteria - GestCell**

Adaptability refers to an interface's ability to serve a variety of users, in Ören and Ghassem-Aghaee's (1994) terminology. GestCell is intended to be useful to users with little knowledge of modelling and simulation techniques. The goal is that GestCell should be useful to users with knowledge from other areas. However, GestCell is also sufficiently sophisticated in modelling and simulation capability that users experienced in modelling simulation will not be slowed down. In fact, GestCell contains the capacity for very complete Gest specifications, but the aspects of Gest not used in simple applications, for example, auxiliary parameters and variables, are hidden from the user. Users who wish to construct very complex models will find GestCell ready to accept these types of elements.

The interface is customizable because all the code for the interface is contained in a file with the Visual Basic® code that can be modified by the user. This also allows the user to maintain the

system because the code is easily available, and Visual Basic for Applications®, found in Excel®, contains facilities for finding the procedures activated by user initiated events.

## **5. Architecture and Functionality of GestCell**

GestCell (Simulation using Gest Environment for Modelling) is a modelling and simulation environment for developing continuous models and performing simulation runs using these models. The system has been developed in response to a need for a modelling and simulation tool in the area of Proton Exchange Membrane Fuel Cell technology. The focus of the development work on the system has been to implement a graphical interface which makes it possible to develop mathematical models and perform simulation runs with very limited experience with simulation languages or methodology. The functionality and architecture of the system will be presented in the following sections. In order to demonstrate the system, a simple pendulum model will be used. However, a sample application of the GestCell tool with a model of the PEMFC is contained in the appendices.

### **5.1 Architecture of GestCell**

GestCell consists of a number of components that are linked to one another. The individual Gest specifications are stored in Excel® workbooks with the extension “.mdl.,” which are linked to another Excel® workbook, which contains the Visual Basic® code for the GestCell procedures. The procedures are activated using a toolbar, a graphical device containing buttons to be clicked by the user, which is attached to the Excel® workbook “refervb.xls,” the workbook containing the Visual Basic® code. New models are created from a template that is activated by GestCell. The simulation runs are carried out using an executable file that is activated from GestCell, and compiled from a C++ file written by GestCell. The program generation is initiated by the user. The individual simulation runs are directed by the system through a file containing information about the selected parameters, initial values and experiments written by GestCell and read by the executable file. The runs are initiated from within GestCell which activates the executable file associated with a model and reads the output from the output files written by the executable file. The information from the workbooks containing the models, parameter sets, initial value sets,

experiments and output data can be passed back and forth from the individual workbooks to “refervb.xls” in order to carry out the GestCell procedures.

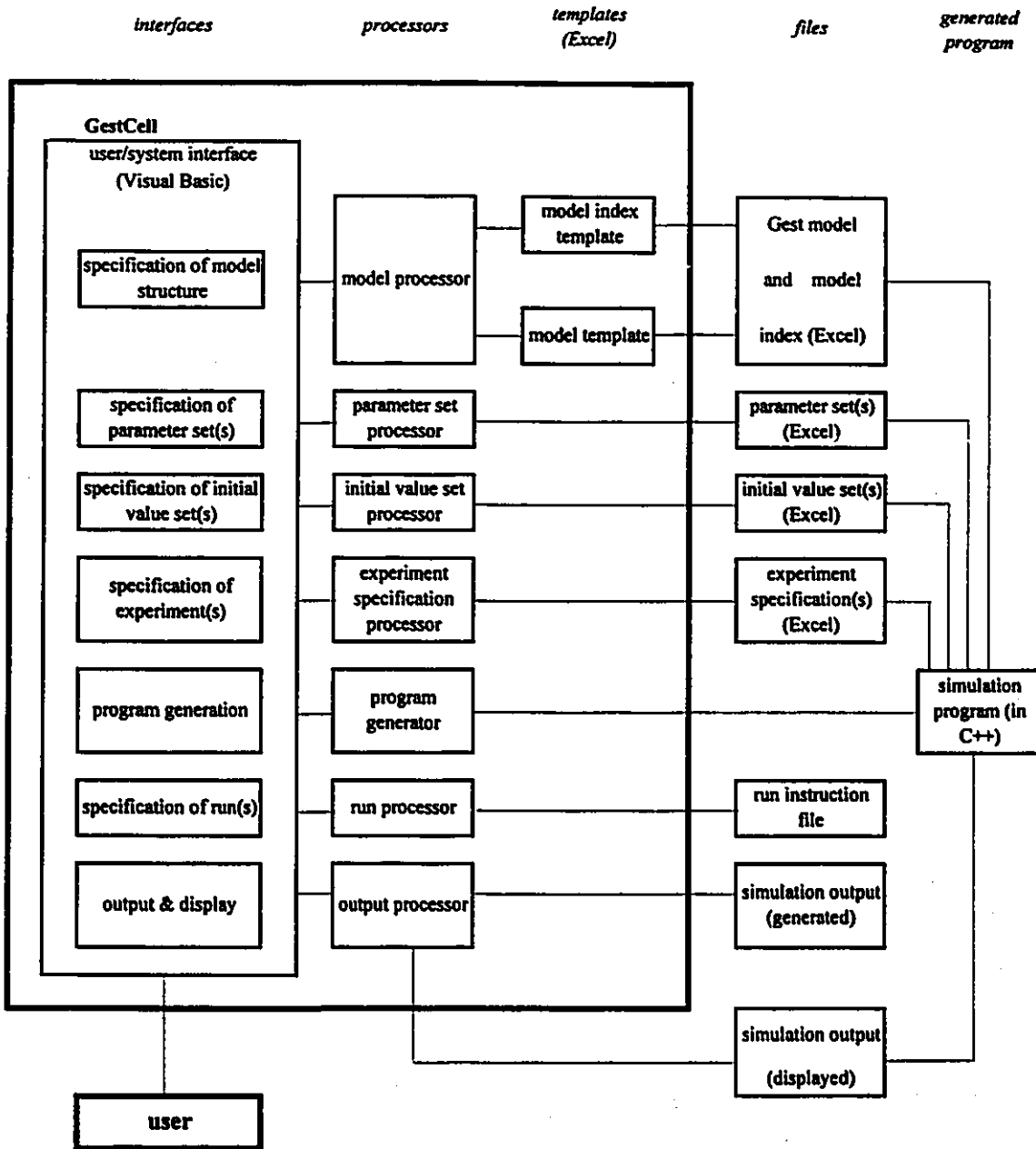


Figure 4. Overall Architecture of GestCell

### **5.1.1 Procedures for Processing the Gest Specification**

As implied by Figure 5, the heart of the GestCell tool is a collection of procedures to handle Gest models which are contained in Excel® workbooks. The Gest specifications are based on a template which is available to the system and is opened in order create a new Gest specification. The Excel® files are activated in the Windows Program Manager using OLE 2.0® (Object Linking and Embedding). This allows a user who is not even familiar with the Excel® spreadsheet package to use the system, because all the necessary files are opened from the GestCell software which is entirely self-contained and is activated from the Program Manager.

When GestCell is activated the file “refervb.xls”, which is an Excel® file containing Visual Basic® code is activated. It is activated by linking it to GestCell using OLE 2.0®. The code contained in “refervb.xls” is linked to any Gest specification workbook that is open in order to handle all the model editing functions, building the C++ files, and handling the output from simulation runs, which can be conveniently stored in the Excel® workbook along with a Gest Specification.

### **5.1.2 Pointers to information in Gest Specifications**

The Gest Specifications are maintained in Excel® workbooks for three reasons:

- pleasant presentation of the Gest specification,
- access to Visual Basic® for interface development
- Access to Excel® procedures such as sorting, parsing, etc. that simplify the handling of the information in the Gest specification, in order to make the interface more powerful.

In order to facilitate the procedures for handling the information in the Gest specification the Excel® workbooks containing the Gest models have a sheet devoted to maintaining a set of pointers for use by the system. The pointers allow insertion and removal of information from the appropriate places as well as a number of sorting and parsing procedures. The information about the Gest specification keeps the system updated as to what information is being displayed or

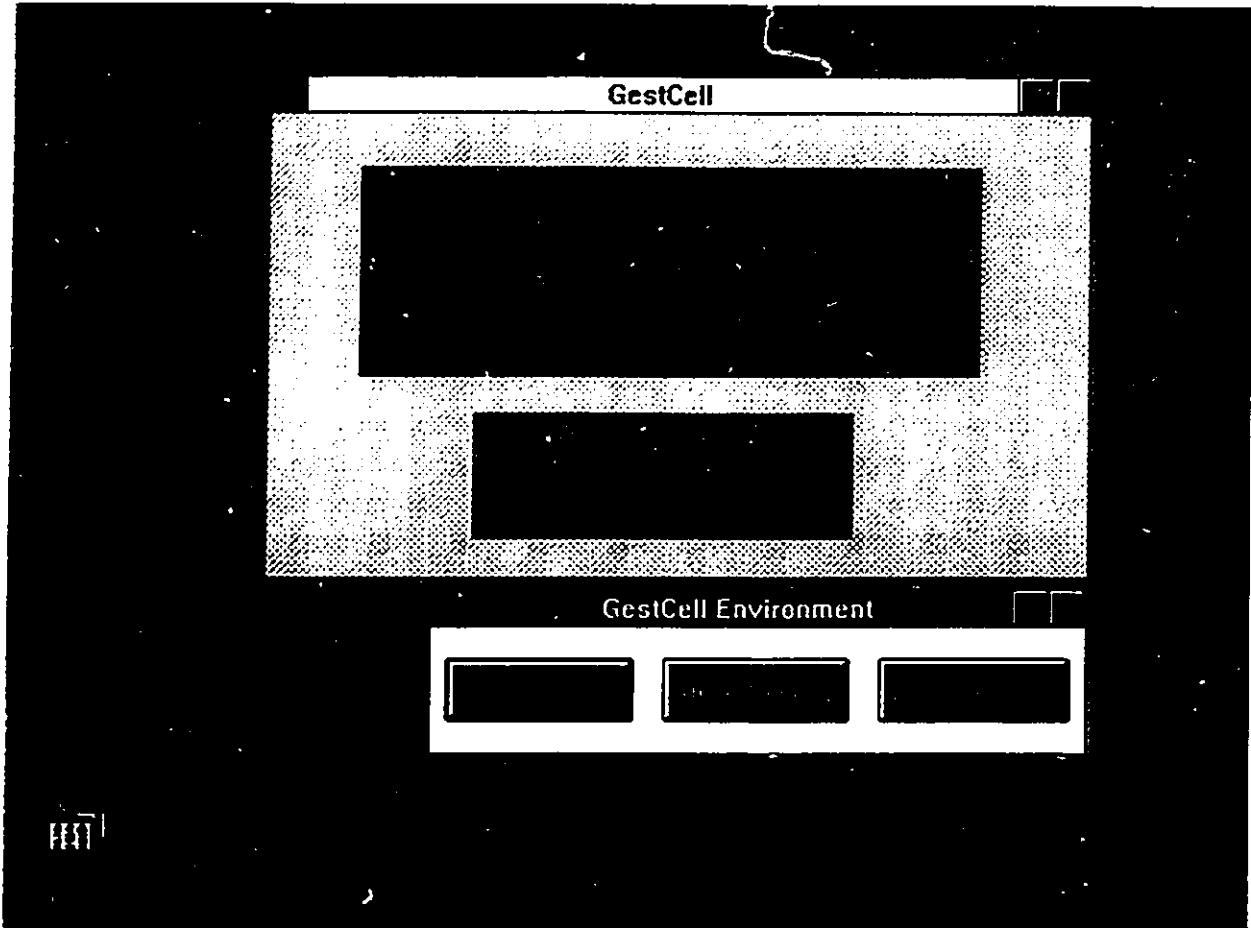
hidden in the Gest specification, as well as locations for particular types of information and amounts of particular types of information. This pointer structure in the Gest workbooks is maintained on an Excel® sheet called “Gest Contents”. The Visual Basic® procedures in “refervb.xls” use the information in the pointer structure, along with the powerful procedures already present in Excel® to process and analyse the information in the Gest specification in a powerful way.

PENDULUM		GEST Specification							
Continuous Model		Pendulum2							
		Example taken from ACSL Beginner's Guide							
Model declarations			hidden	Starts at row	# of entries				
	Independent variable	No		9	1				
	Input variables	Yes		11	0				
	Output variables	No		12	1				
	State variables	No		14	2				
	Auxiliary variables	Yes		17	0				
	Constants	No		18	2				
	Parameters	No		21	3				
	Auxiliary Parameters	Yes		25	0				
	Tabular functions	Yes		26	0				
	Interpolated variables	Yes		27	0				
Dynamic									
	Input variables	No		29	0				
	Auxiliary variables	Yes		30	0				
	Derivatives	No		31	2				
	Output functions	No		34	1				
						# of Items			
Parameter Sets		No		38	3	3			
Initial Value Sets		No		56	2	2			
Experiment(s)		No		66	1	min items	+items(1)	+items(2)	+items(3)
						13	2	0	0

Figure 5. Pointer structure attached to Gest specifications in GestCell

## 5.2 Using GestCell

As mentioned above GestCell is completely self-contained and is activated from the Program Manager in Windows®. At that time the user can choose to open a new model or an existing model.



**Figure 6. GestCell at start up.**

A simple pendulum model has been implemented in GestCell for demonstration purposes, so at this time the user can open the file by selecting "Open Model..."

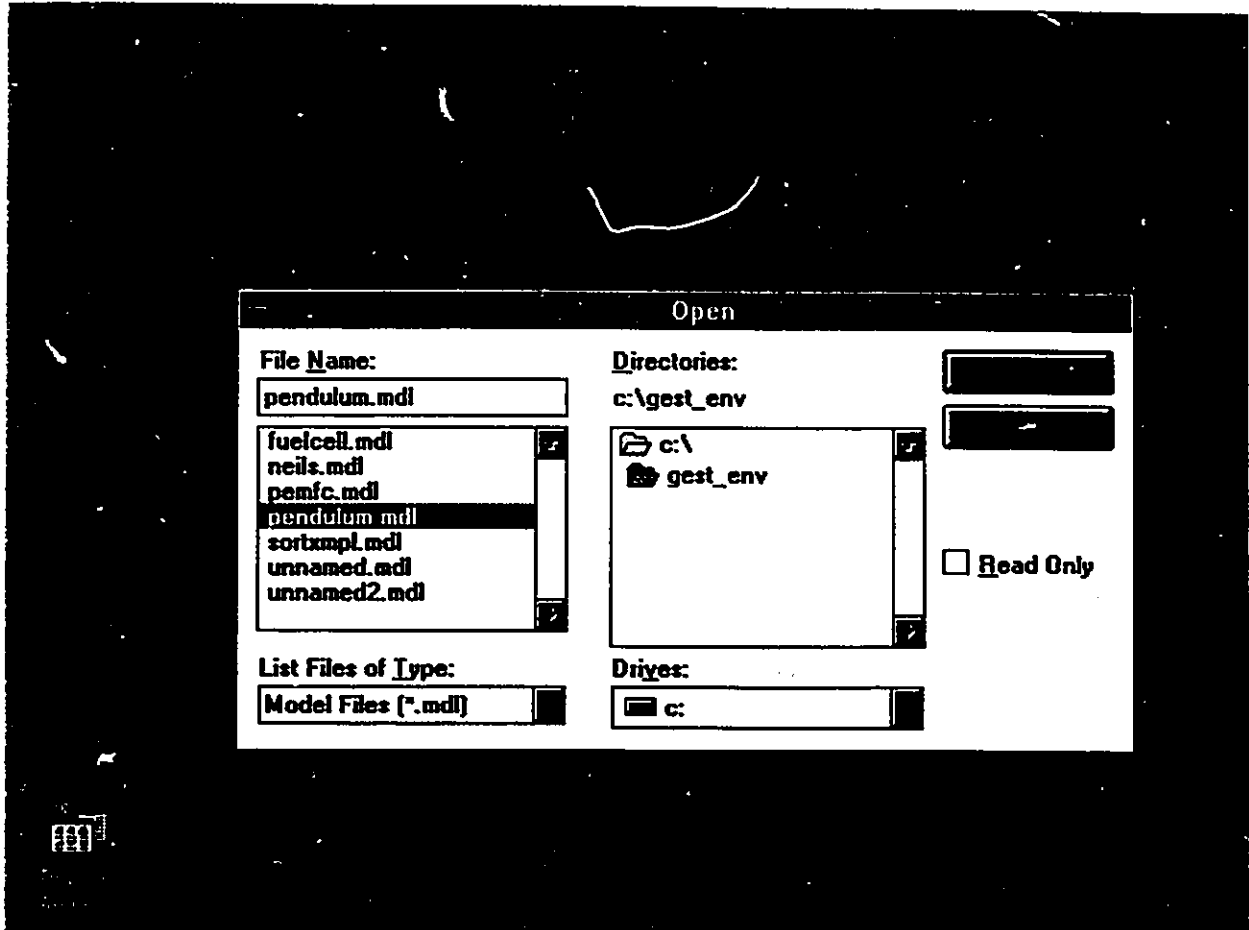


Figure 7. Opening an existing Gest Specification.

As can be seen the user selects a file from the standard file open dialog box. The dialog is set to look in the home directory of GestCell. In the figure above the file "pendulum.mdl" has been selected. Using the pendulum example the important functions of GestCell will be demonstrated.

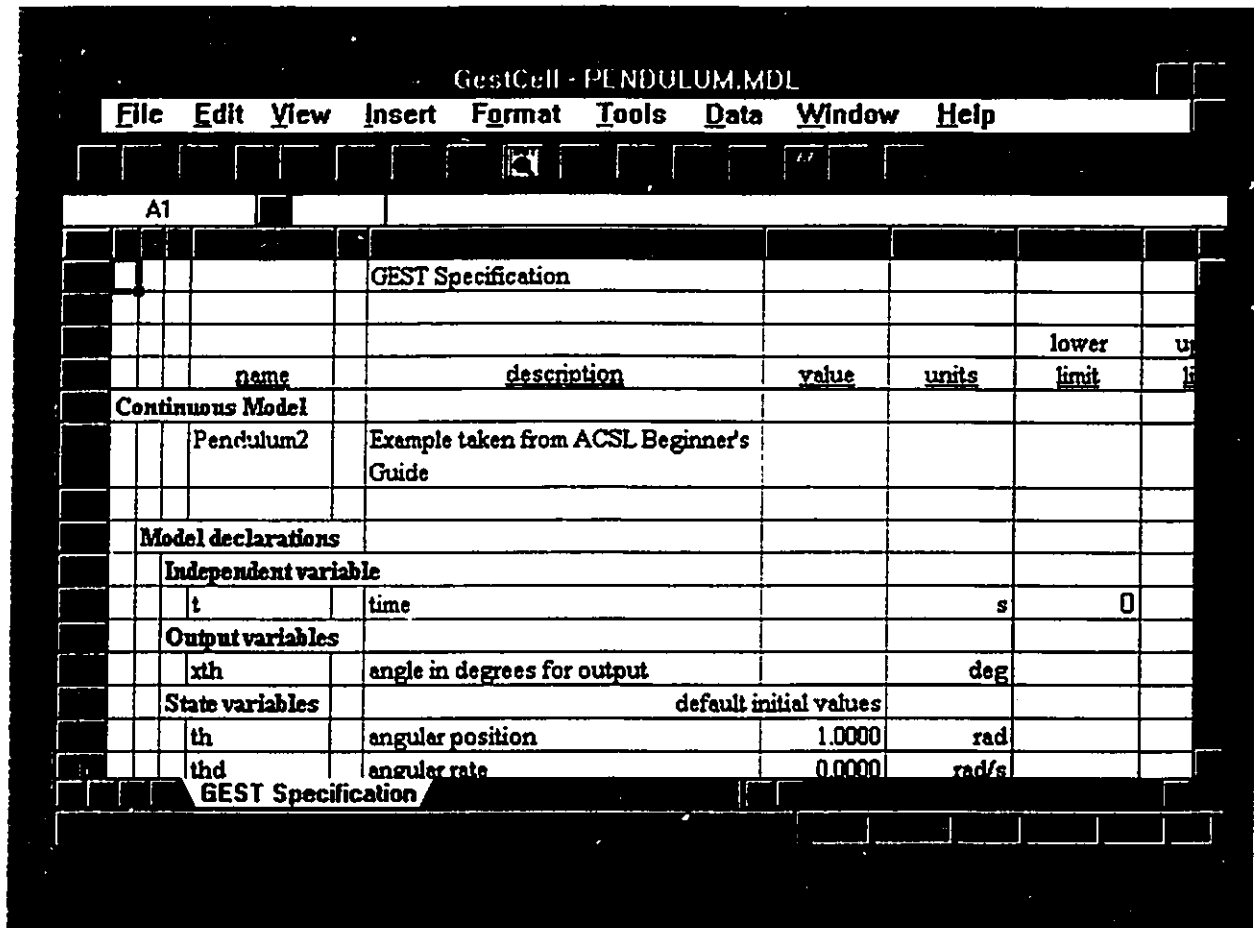


Figure 8. GestCell interface in Excel®

Upon opening a Gest Specification in GestCell, the user can perform any modelling and simulation task using a custom toolbar, a graphical device containing buttons to activate procedures, designed for GestCell and attached to "refervb.xls," which is the workbook containing the Visual Basic® code for the GestCell procedures.

Although the custom toolbar is not plainly visible in the picture, it allows the user to move step by step through the Gest specification and the simulation runs and analysis. In the interest of naturalness (Ören and Ghasse-Aghaee, 1995), the toolbar buttons are organized in an order that leads the user through the entire procedure. The buttons appear on the toolbar as follows:

- open new model button, allowing the user to open a new model

- name model button, allowing the user to give a name to the model
- open model button, allowing the user to open an existing model
- add model element button, allowing the user to add elements to the mathematical model
- edit model button, allowing the user to edit model elements in the mathematical model, the reasons for keeping add and edit separate will be explained below
- parameter sets button, allowing the user to specify any number of parameter sets, edit the sets by individual parameter value
- initial sets button, allowing the user to specify initial value sets, edit the sets by individual initial value
- experiment button, allowing the user to specify any number of experiments and edit the experiments
- output button, allowing the user to specify the output from any particular experiment
- Gest → C button, allowing the user to build the C++ program and compile it for running simulation experiments
- go button, allowing the user to specify individual simulation runs
- get data button, allowing the user to import output data from simulation runs into the Gest specification
- graphs button, allowing the user to specify graphical output, including comparison of different runs
- standard printer button, allowing the user to print any part of the Gest specification workbook
- standard save button
- exit button, allowing the user to exit GestCell, closing all the files opened by the system

### **5.2.1 Editing Gest Specifications**

Upon clicking the Add or Edit toolbar buttons the same dialog box will appear but with slightly different appearance. Depending on whether the user wishes to add model elements or edit existing model elements the dialog box works differently. This might at first seem an unnatural separation of the two functions. Normally, when developing a model, the activities of adding and editing elements to a model are distinct, even if adding consists only of declaring the

variables, for instance. During model development, editing is the primary activity with respect to model elements. Because these two activities are treated separately in GestCell, there are a number of features that make the system more effective for the user.

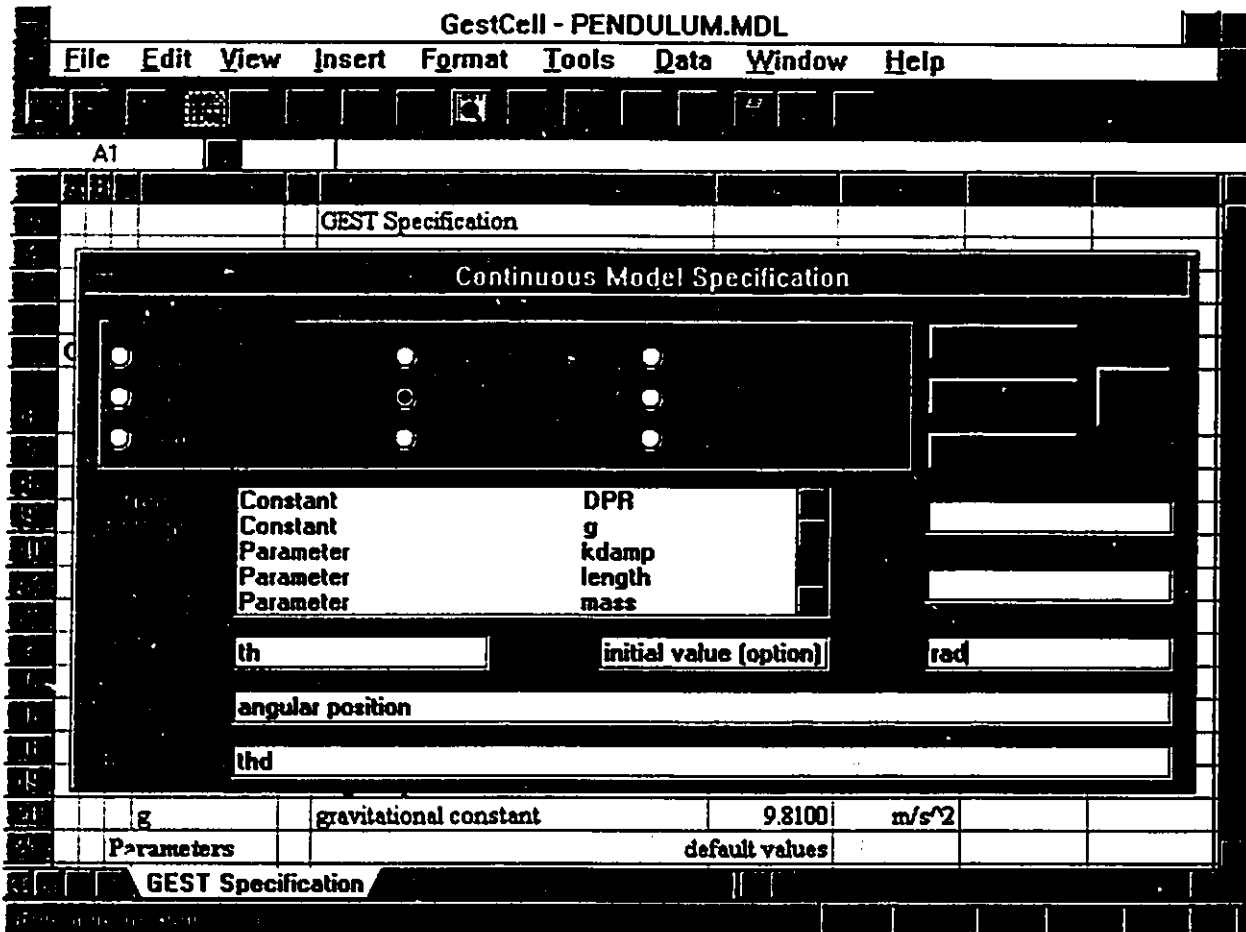


Figure 9. Editing Dialog box displayed after pressing the Add toolbar button

The dialog box above is displayed upon pressing the “Add” toolbar button, and the identical dialog

box is displayed upon pressing “Edit”. When adding an element to the model, the user specifies the type of element using the option buttons on the top of the form. Using edit boxes, the user gives some or all of the following information for a model element: name, value (default value for initial values, parameters and constants), units, lower limit, upper limit, description and

equation. To prevent errors entering the equations, the label next to this edit box shows all the information, except the right hand side of the equation that is the label reads “[name] = ” or “[name] ’ = ”. To further prevent errors in equations, all the model elements are displayed in a list box on the form, along with the type of element, and clicking on an element in the list box inserts the element into the equation edit box to prevent typographical errors. When finished entering the information the system inserts all the information into all the appropriate places in the Gest specification, including declarations, dynamics, parameter sets and initial value sets.

When the user selects “Edit,” the same dialog box functions differently. The option buttons for specifying the type of element are disabled. The list box containing the model elements is used to select a model element. When an element is selected, all the information in the model for the element is displayed in the edit boxes, and the user is able to edit any piece of information.

When the user is finished, the system will update the information throughout the Gest specification after confirmation with the user. The user may also delete any model element from this dialog box, after all the information about the element has been displayed and the user confirms the delete command.

### **5.2.2 Specifying Parameter and Initial Value Sets**

As mentioned in the previous chapter, a Gest specification consists of a mathematical model as well as parameter sets, initial value sets and experiment specifications. The parameters and state variables are inserted and edited using the dialog box discussed above. The user may edit parameter sets or initial value sets at any time by pressing the toolbar buttons “Prmt” or “Init”. In the interests of consistency for the user, the editing dialog boxes for both parameter sets and initial value sets function exactly the same way. Therefore, only the parameter set dialog will be discussed below.

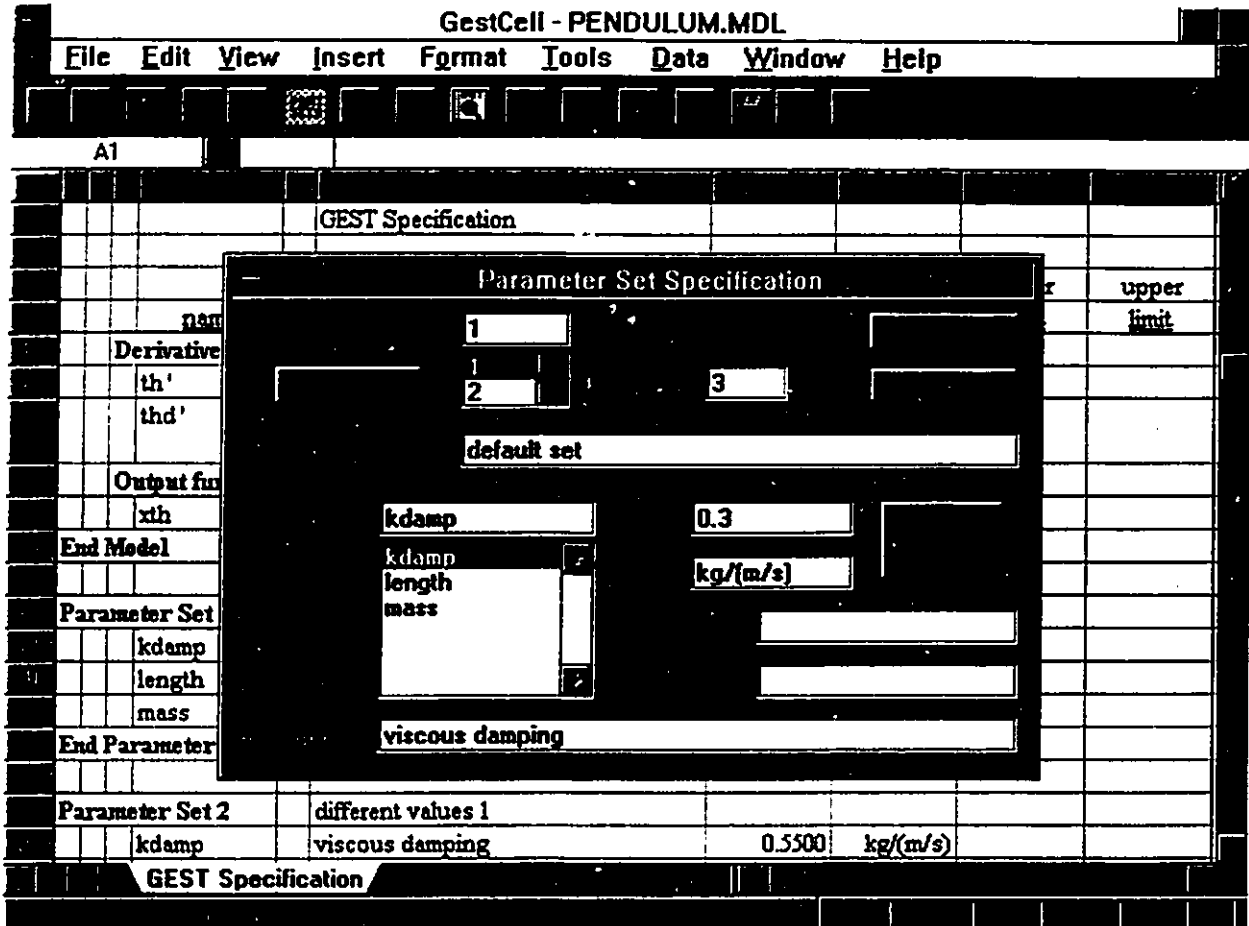


Figure 10. Parameter set dialog box

The parameter (and initial value) dialog box has two distinct areas separated by a line. On the top half of the dialog, the user selects a particular set to edit, and the description of the set is displayed as further information about the set. The description may be edited in order to ensure the description is appropriate for the set. The user may also choose to specify a new set, which is a copy of the default set that may be edited. On the bottom half of the dialog, a list box contains all the parameters (or state variables) in the model. When the user selects a particular element from the list box all the information about the element is displayed, including the value in the set, lower limit, upper limit, and description. The user may edit and insert individual values into the set being edited. When a new value is inserted, the element is removed from the list box, which prevents the user from unnecessarily or mistakenly editing the same value in a set

twice. In large sets of parameters or initial values, it also provides a way for the user to be sure every value in the set has been set. The list box will be empty if every value has been set.

### 5.2.3 Editing Experiment Specifications

The final part of a Gest specification is the specification of the simulation experiment. Note that a simulation experiment is not the same as a run. The experiment is a set of experimental parameters such as initial and terminal values for the independent variable, step size and communication interval and the numerical method.

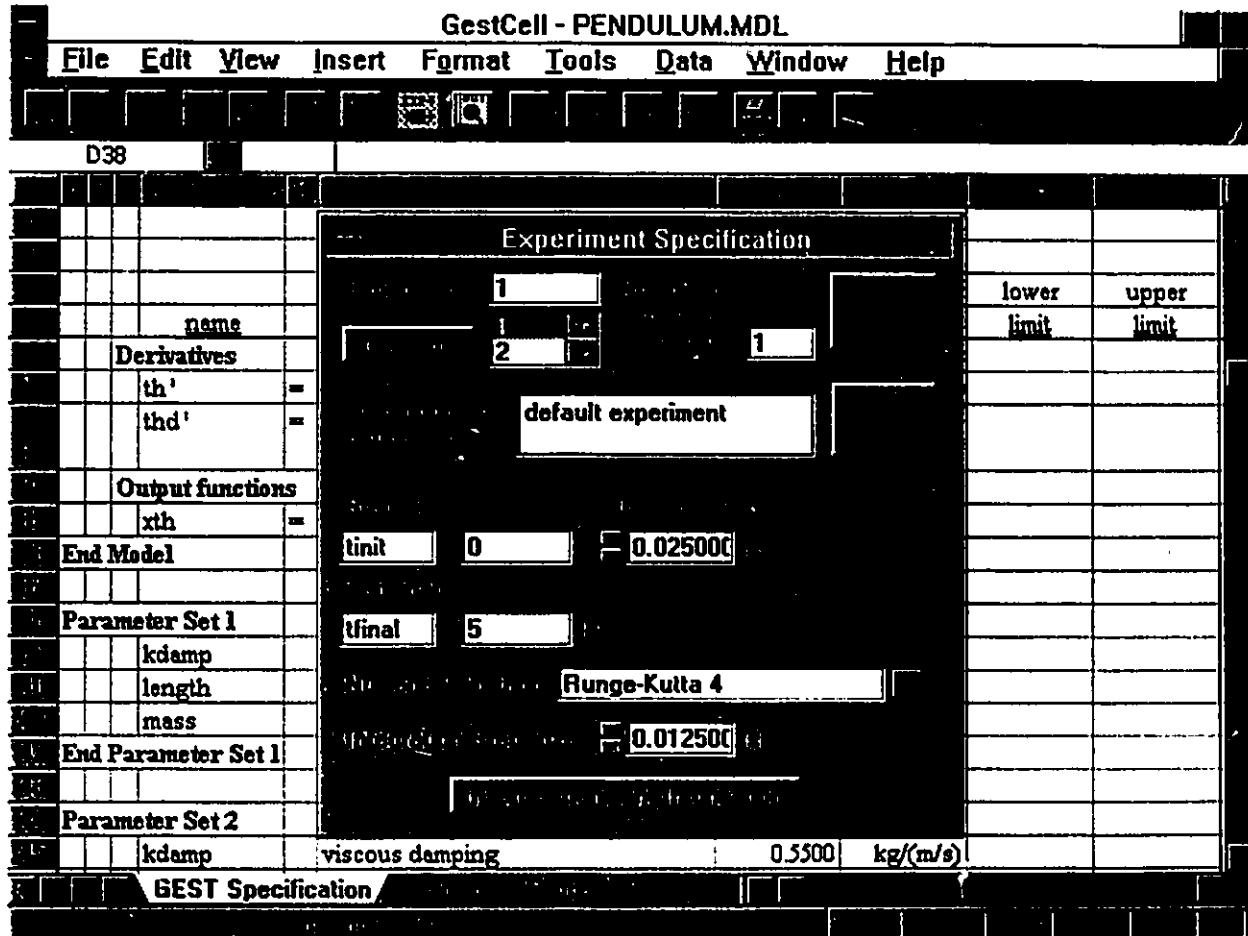


Figure 11. Experiment specification dialog box

Similarly to the parameter and initial value dialog boxes, the experiment dialog box is split into two parts for selecting the experiment to edit, and editing the information contained in the selected experiment specification. When a user is finished editing the information, it is inserted into the appropriate places in the appropriate experiment.

Another part of any experiment specification in Gest is the specification of the model elements to be stored as output from the simulation run. GestCell retrieves this information from a separate dialog box, in order to keep the experiment dialog box from becoming too cluttered.

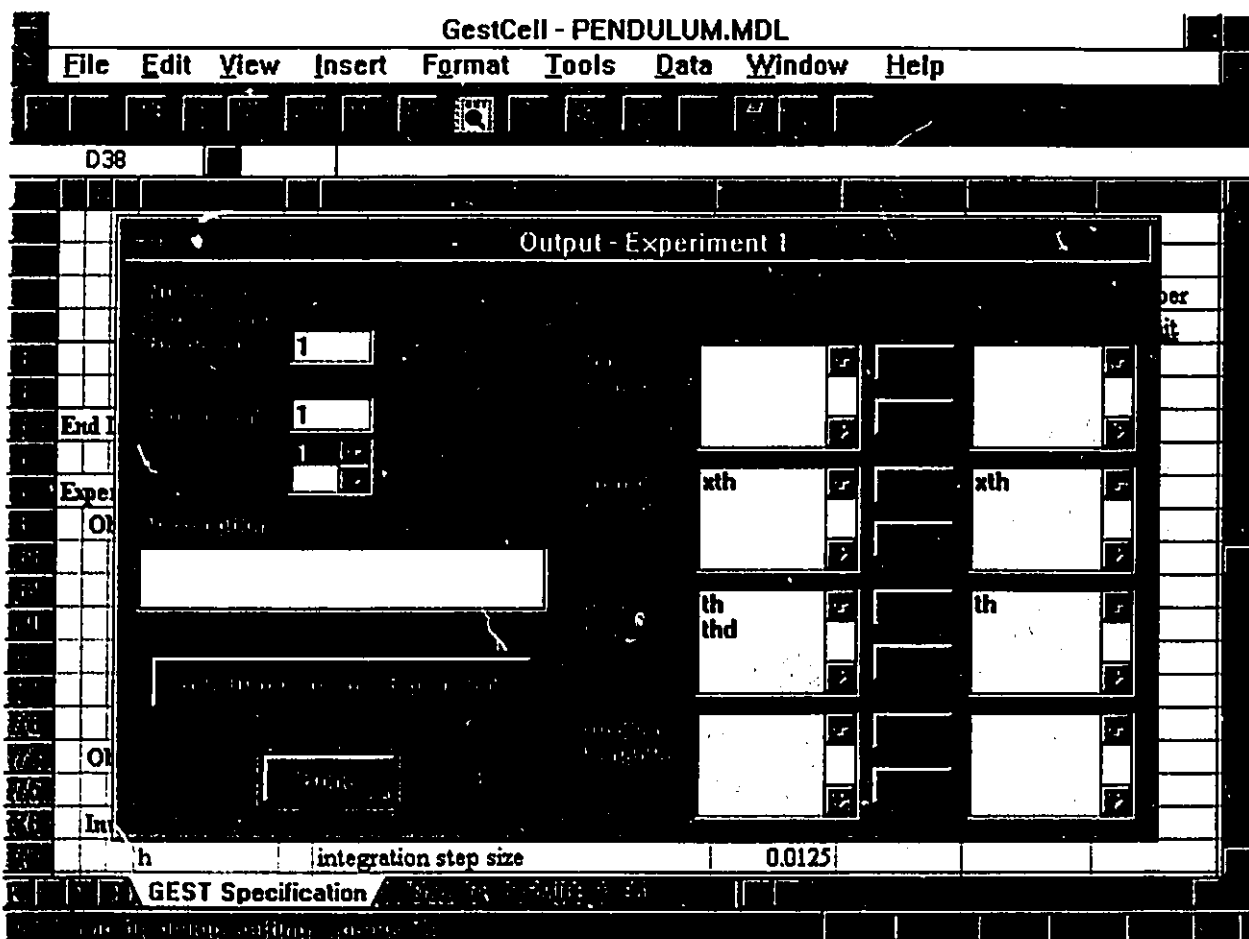


Figure 12. Output dialog box

Again this box allows the user select a particular experiment. All the variables in the model are listed in boxes and the user can add or remove the variables from list boxes that specify the

output for the particular experiment. When the user has selected all the variables for output, they are inserted into the appropriate places in the experiment specification.

The experiment specification is the final part of a Gest specification. With the underlying model specified, and the associated parameter, initial value and experiment information, the user may compile the Gest specification to a C++ file, which is compiled to an executable file. A simulation run can then be performed, with any combination of parameter set, initial value set and experiment, using the simulation dialog box in GestCell.

#### **5.2.4 Generating the Executable File for Simulation Runs**

The Gest specification that has been constructed with information from the user GestCell will analyse the contents of the Gest specification and generate a C++ file, named "Gestsim.cpp." GestCell enters all the parameter sets, initial value sets and experimental parameter sets into a file named, "Gestsim.h" which is referenced in "Gestsim.cpp" allowing the user to perform runs using any values from any of the sets in the Gest specification. GestCell also generates a file named "Gestout.h" which contains sets of integers that are either "0" or "1" which instructs the executable file as to which variables to output for a particular simulation run, based on the experiment selected. The numerical methods are programmed as a C++ class and are included in "Gestsim.cpp" as a header file, "nummeth.h", which allows the user to perform simulation runs using different numerical methods without recompiling the executable file.

Simulation programs have been generated in C, in the past by processing a Gest specification (Qiang, 1993). However, the processing used to construct the C++ program in this case is novel for two reasons. First the interface is intended to construct the Gest specification in an identical manner every time, which ensures the specification conforms to the proper format. Second, the pointer structure provides information to the system about where particular model elements are found in the specification, which facilitates generating the C++ file.

GestCell uses the sorting, parsing and searching features of Excel® in the analysis of the Gest specification, in order to sort all the auxiliary variables during program generation, as well as altering the formulas for the derivatives to use the internal variables used in “nummeth.h” and generating the file “Gestsim.h” and “Gestout.h.”

The entire program generation is activated by clicking on the “Gest → C” toolbar button, which, upon confirmation from the user, generates the files, “Gestsim.cpp,” “Gestsim.h,” and “Gestout.h.” The file “Gestsim.cpp” is then compiled to a file named “[model name].exe” so that each Gest specification has an associated executable file.

### **5.2.5 Performing Simulation Runs**

As mentioned earlier, individual simulation runs in Gest are specified by selecting a parameter set, an initial value set and an experiment. GestCell contains a dialog box to elicit this information from the user.

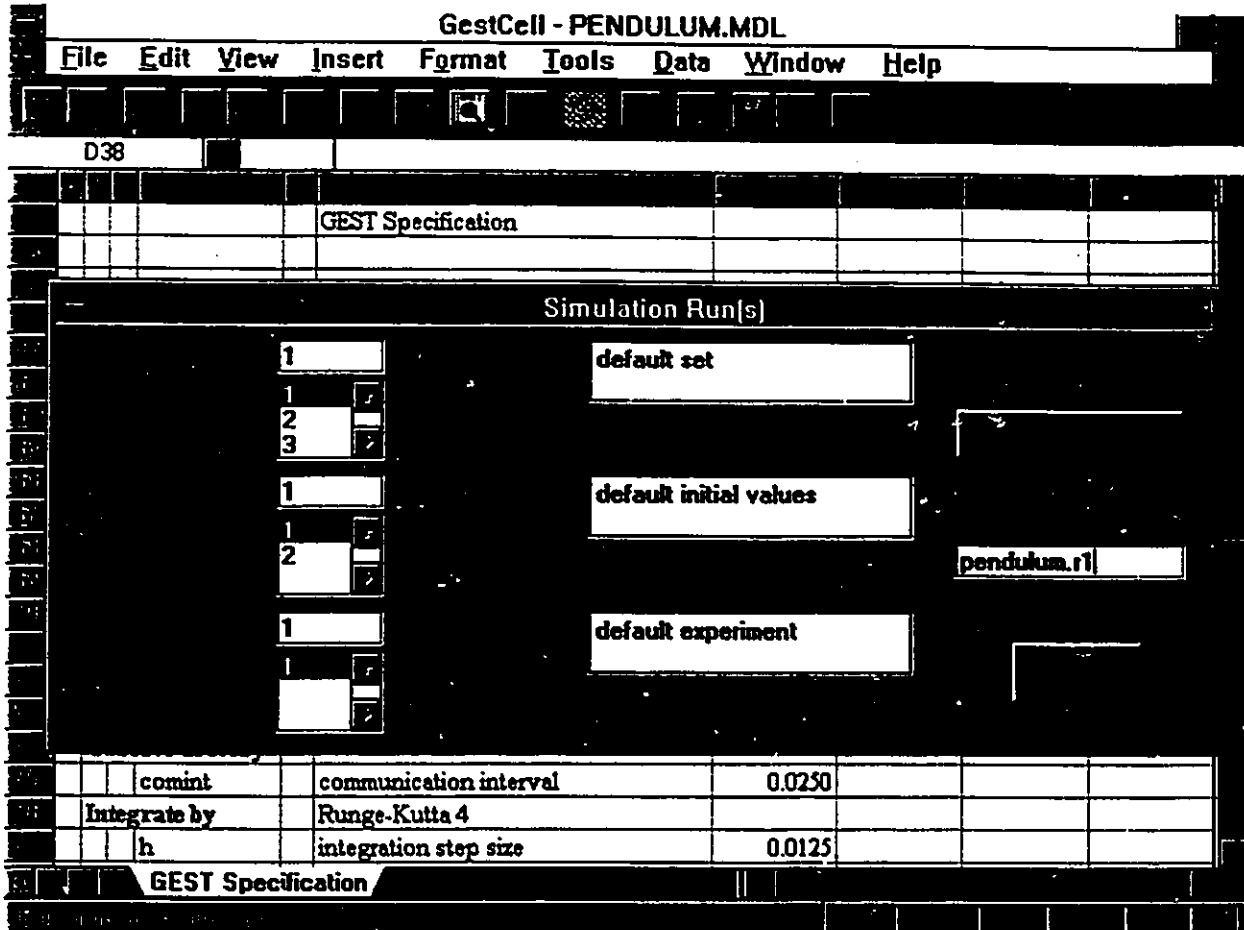


Figure 13. Simulation dialog box

The dialog box contains lists of all the parameter sets, all the initial value sets and all the experiments in the Gest specification. The user must also specify the filename for the output from the simulation run. When the user clicks the “Perform Simulation” button the system writes a file, “[model name].run” which contains the number for the parameter set, initial value set and experiment as well as the name of the output file. The executable file is activated, which retrieves all the information it needs from “[model name].run” in order to perform the simulation run. The output is written to the specified file as comma-delimited text which can easily be imported into GestCell.

### **5.2.6 Retrieving and Analysing Output Data**

At any time, the user may import output files from simulation runs into the workbook containing the Gest specification. The toolbar button “Get Data” is used for this purpose, and after selecting a file from a standard file dialog box the comma-delimited text file is imported and inserted on a worksheet with the time and date. The user may generate graphs using the Excel® graphing capabilities or the GestCell toolbar button “Graphs,” which allows the user to select data sets for graphs using list boxes.

### **5.3 A Gest Specification Constructed Using GestCell**

The interface of GestCell is intended to produce Gest specifications of systems by eliciting from the user all the necessary information and constructing the specification. As mentioned above, GestCell is able to generate a C++ program for carrying out simulation runs. Clearly then, Gest is sufficiently systematic in its structure for the computer to be able to interpret it for simulation purposes. However, the GestCell system also uses the Gest specification as documentation of a mathematical model. The dialog boxes are designed to retrieve the information for a complete Gest specification, with no more nor less information required from the user. Therefore the Gest specification itself is an important part of the GestCell interface, since the user should be able to read the Gest specification and interpret the model correctly as well as use the Gest specification for documentation purposes when communicating the model to others.

### GEST Specification

name	description	value	units	lower limit	upper limit
<b>Continuous Model</b>					
Pendulum2	Example taken from ACSL Beginner's Guide				
<b>Model declarations</b>					
<b>Independent variable</b>					
t	time		s	0	
<b>Output variables</b>					
xth	angle in degrees for output		deg		
<b>State variables</b>					
		default initial values			
th	angular position	5.0000	rad		
thd	angular rate	0.0000	rad/s		
<b>Constants</b>					
DPR	degrees per radian - for conversion	57.2958	deg/rad		
g	gravitational constant	9.8100	m/s <sup>2</sup>		
<b>Parameters</b>					
		default values			
kdamp	viscous damping	0.3000	kg/(m/s)		
length	length of the rod	0.5000	m		
mass	mass of the pendulum	1.0000	kg		
<b>Dynamic</b>					
<b>Derivatives</b>					
th'	= thd + t		rad/s		
thd'	= -(mass * g * sin(th) + kdamp * length * thd) / (length * mass)		rad/s <sup>2</sup>		
<b>Output functions</b>					
xth	= DPR * th		deg		
<b>End Model</b>					

**Figure 14. Gest specification of a pendulum model constructed using GestCell**

```

Parameter Set 1      default set
  kdamp              viscous damping      0.3000  kg/(m/s)
  length            length of the rod     0.5000  m
  mass              mass of the pendulum  1.0000  kg
End Parameter Set 1

Parameter Set 2
  kdamp              viscous damping      0.5500  kg/(m/s)
  length            length of the rod     0.6000  m
  mass              mass of the pendulum  1.0000  kg
End Parameter Set 2

Parameter Set 3
  kdamp              viscous damping      0.5000  kg/(m/s)
  length            length of the rod     1.0000  m
  mass              mass of the pendulum  0.1000  kg
End Parameter Set 3

Initial Value Set 1  default initial values
  th                angular position     1.0000  rad
  thd               angular rate        0.0000  rad/s
End Initial Value Set 1

Initial Value Set 2  different values
  th                angular position     0.9000  rad
  thd               angular rate        0.0000  rad/s
End Initial Value Set 2

Experiment 1        default experiment
  Observe
    Output variables
      xth
    State variables
      th
    Observe at every
      comint         communication interval  0.0250
    Integrate by
      h              Runge-Kutta 4
      h              integration step size   0.0125
    Start at
      tinit          initial time           0.0000
    Terminate when t >=
      tfinal         time condition         5.0000  s
End Experiment 1

```

Figure 15. Gest specification of pendulum model parameters, initial values and experiment

As can be seen in the above figures, the Gest specification constructed by GestCell is quite readable and provides a very informative model for the user. In fact, the Gest specification is sufficiently informative, as to have provided no facility for comments in a GestCell simulation model because part of the Gest specification in GestCell allows the user to input a description for every model element, as part of the model.

The Gest specification itself, coupled with the graphical interface in GestCell, provides the user with a great deal of information at all times that may be used in model development. The example in the listing above is a simple system, but complex systems such as PEMFCs must be modelled using a large number of variables and relationships. In complex systems GestCell provides the user with a powerful way to organize a model, and model development is facilitated by the Gest specification.

Parameter Set				1	
Initial Value Set				1	
Experiment				1	
Communication Interval				0.025	
Number of Points				201	
Point	t	xth	th	thd	
0	0	57.2958	1	0	
1	0.025	57.0008	0.994851	-0.410855	
2	0.05	56.121	0.979496	-0.815895	
3	0.075	54.6666	0.954113	-1.21233	
4	0.1	52.6521	0.918953	-1.59722	
5	0.125	50.0963	0.874346	-1.96736	
6	0.15	47.0227	0.820701	-2.31928	
7	0.175	43.4601	0.758521	-2.64923	
8	0.2	39.4427	0.688405	-2.95318	
9	0.225	35.0108	0.611053	-3.22698	
10	0.25	30.2105	0.527273	-3.46643	

Figure 16. Top of output data generated using GestCell (pendulum model)

In the above figure, the top of the output data generated from the pendulum model in GestCell is shown. The data was generated by activating a simulation run using the “Go” toolbar button and selecting parameter set 1, initial value set 1 and experiment 1 as indicated on the top of the file.

Following the run, the output file was imported into the Excel® workbook containing the pendulum model, “pendulum.mdl,” using the GestCell toolbar button, “Get Data.”

#### **5.4 Simulation of the PEMFC Using GestCell**

GestCell has been used to perform some simulation using a simple dynamic model of a PEMFC. The dynamic model of a PEMFC presented in the appendix is under development. There are a number of simplifying assumptions made throughout. The density of gases and partial pressures, as well as the calculation of cell voltage are probably the interesting components of the model. The energy balances are not included at this stage.

The model follows the structure set out by He (1994a, 1994b), for a dynamic model of a molten carbonate fuel cell. The differential equations take a similar form as in He’s work (1994b), and represent conservation equations as described in Chapter 2. The calculation of cell voltage uses equations given by Koene et al. (1993). The differential equations for mass balances effect the partial pressures of the gases in the model, which in turn effect the cell voltage. Regulation of pressure has been assumed, so that in time the cell will always return to a desired pressure in each of the gas feedstreams. The temperature of the cell and the gases have been assumed constant.

The model described above has been used to simulate the case where a cell with a current density of  $0.0 \text{ A/cm}^2$  is stepped up to a current density of  $0.5 \text{ A/cm}^2$ . In figures 17 and 18 below, it can be seen that this increase in voltage results in an increase in the partial pressures of the gases. The feed rates of the gases to the cell have been modelled as proportional to the current density. The voltage of the cell drops as a result of the increased current, which is expected. The model quickly reaches a steady state.

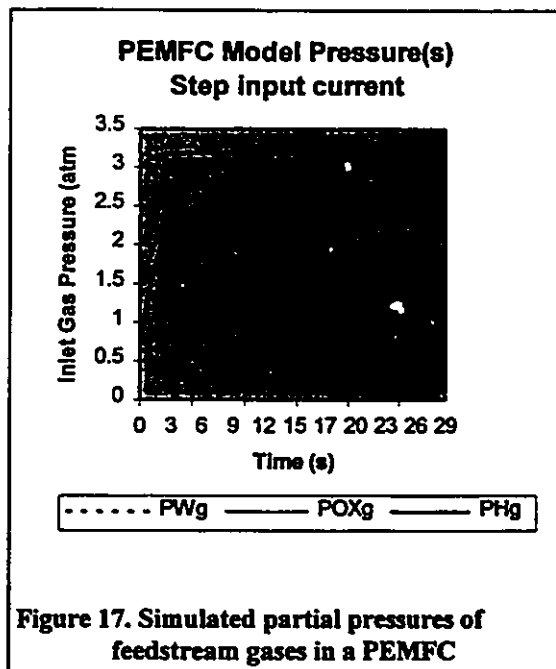


Figure 17. Simulated partial pressures of feedstream gases in a PEMFC

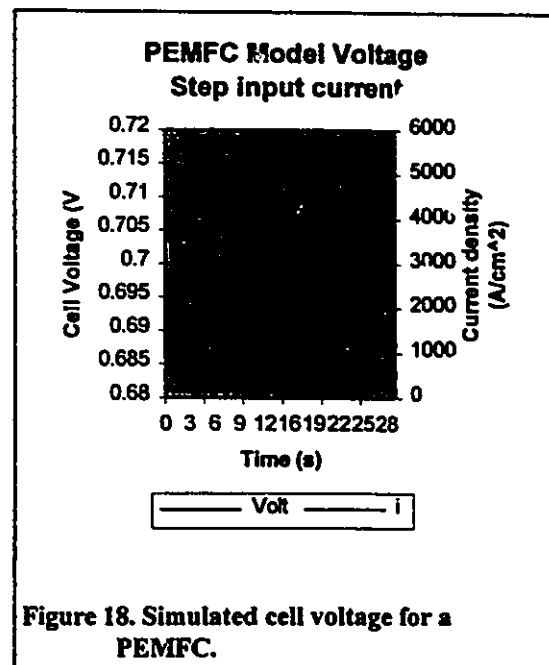


Figure 18. Simulated cell voltage for a PEMFC.

This dynamic model of the PEMFC has not been validated and is in need of further development. However, the results of the simulation run presented here appear to be reasonable, and the cell voltage of roughly 0.7 V at 0.5 A/cm<sup>2</sup> is realistic. In addition to the change in the steady-state value of the voltage for a PEMFC, the graphs clearly show a transient response to a step increase in current. The steady state voltage is reached when the partial pressures of the gases reach a steady state at the new feed rates. Temperature changes would also effect the voltage of the cell, but have not been included.

These graphs represent a single simulation run of this model in GestCell. The model in the appendix shows that even this simple consideration of a dynamic model has a large number of variables and is complex. The complexity of PEMFC systems can be better understood and improved through continued simulation efforts, and GestCell has the potential to provide a modelling and simulation tool for this purpose.

## **6. Conclusions and Future Work**

This thesis summarizes the research carried out with regards to two main topics. Modelling and simulation of the proton exchange membrane fuel cell (PEMFC) is the first topic addressed in the work and serves as a motivation for the second part. A modelling and simulation system, GestCell, has been developed with particular consideration given to making model specification and simulation transparent to users who may not be familiar with simulation methodology.

### **6.1 Achievements**

The PEMFC is a promising technology for clean energy conversion in the future. In surveying the existing literature and considering a number of the issues related to dynamic models of PEMFCs in general, it is suggested that dynamic simulation of the PEMFC is achievable. The simulation that has been done in the area is not voluminous but does succeed in simulating the steady-state behaviour of the PEMFC. Drawing on the insights contained in the steady state models, dynamic models should be forthcoming. The biggest difficulty facing simulation of the PEMFC seems to be the relatively small number of scientists knowledgeable about the technology who conduct simulation. It is hoped that the survey and comments in the thesis will help to motivate further work in simulation of PEMFCs

The most promising accomplishment of the research for this thesis has been the development of the GestCell system, for users who are not experienced in simulation or programming. GestCell has a number of features that hold potential for future use in modelling and simulation research, including the GestCell interface and the pointer structure used in processing the specifications.

The GestCell interface is implemented in Visual Basic® within the Excel® spreadsheet package. GestCell has a graphical interface that allows non-programmers to develop complete Gest specifications and perform simulation runs.

GestCell has a pointer structure used for processing the specifications that provides a great deal of information about the types of model elements in a specifications as well as the location of particular information within the specification. This type of information allows GestCell to use the powerful searching, sorting and parsing facilities within Excel® to process the specifications effectively.

A Gest specification in Excel® is a highly readable presentation of a mathematical model and GestCell is able to process such a specification to generate a C++ program in order to carry out simulation runs.

GestCell is a complete modelling and simulation environment. The user is able to specify a mathematical model through a friendly and powerful interface that transparently provides the ability to conduct simulation with the specification. Furthermore, GestCell is accessible to non-programmers but also has the ability to handle large, interesting systems. As such GestCell attempts to make simulation more widely available to all sorts of users.

## **6.2 Future Work**

In future it is hoped that GestCell will allow non-traditional users of simulation to develop mathematical models and benefit from simulation. In particular, it is hoped that modelling and simulation of PEMFCs will be undertaken more widely and at advanced levels. Future development of dynamic models of PEMFCs and simulation studies would help to advance a promising clean energy technology.

The simulation of PEMFCs will require more flexible numerical methods and simulation abilities than GestCell currently has. GestCell has a numerical library with four fixed step numerical methods, the most sophisticated of which is Runge-Kutta 4th order method. However, it was found, in efforts to model the PEMFC, that stiffness and accuracy can be problematic. This is of

course true for many other systems as well, and GestCell would be greatly improved with the ability to handle stiff and discontinuous systems.

GestCell could be made much more powerful by developing an extensive knowledge base. There is presently some very basic consistency checking, such as ensuring that all parameter and initial values are set. However, a variety of consistency checks and error handling procedures would make GestCell much more powerful. Furthermore, GestCell is currently implemented with only one template for the Excel® workbooks. Continuous models are the only type of models that GestCell currently supports. With a variety of templates, GestCell's abilities could be greatly enhanced. Finally, tabular functions have not been implemented in GestCell. The ability to handle user-specified tabular functions would be an asset, and a library of tabular functions and constants stored in an Excel® workbook would be a straightforward way to make a great deal of knowledge available in GestCell.

## References

- ACSL Beginner's Guide 10.1, "Example 2 Pendulum," Mitchell & Gauthier Associates Inc., Concord, MA
- Amphlett, J.C., Baumert, R.M., Mann, R.F., Peppley, B.A. and Roberge, P.R. (1993), "A Performane Model for PEM Fuel Cells." Proceedings of the 28th Intersociety Energy Conversion Engineering Conference, The American Chemical Society, Washington, D.C., Vol. 1, pp. 1215-1226.
- Anahara, R. et al. (1993), "Present Status and Future Prospects for Fuel Cell Power Systems," Proceedings of the IEEE, 81: 3 (March), 399-408.
- Bagotsky, V.S. & Skundin A.M. (1980), Chemical Power Sources, Academic Press, New York, pp.342-3.
- Beek, W.J. & Mutzall, K.M.K (1975), Transport Phenomena, John Wiley & Sons Ltd., Toronto.
- Bernardi, D.M. & Verbrugge, M.W. (1992), "A Mathematical Model of the Solid-Polymer-Electrolyte Fuel Cell," Journal of the Electrochemical Society, 139: 9 (Sept.), 2477-2491.
- Bernardi, D.M. (1990), "Water-Balance Calculations for Solid-Polymer-Electrolyte Fuel Cells," Journal of the Electrochemical Society, 137. 11 (Nov.), 3344-3350.
- Britz, Dieter (1981), Lecture Notes in Chemistry, Springer-Verlag, New York.
- Broadhead, J. (1984), "Electrochemical Principles and Reactions," chapter 2, Handbook of Batteries and Fuel Cells, McGraw-Hill Book Company, New York, New York, pp.1-34.
- Fickett, A.P. (1984), "General Characteristics," chapter 41, Handbook of Batteries and Fuel Cells, McGraw-Hill Book Company, New York, New York, pp.3-15.
- Fry, M.R. (1993), "Environmental Impacts of Electricity Generation: Fuel Cells," IEEE Proceedings-A, 140: 1 (Jan.), 40-1.
- Fuller, T.F. & Newman, J. (1993), "Water and Thermal Management in Solid-Polymer-Electrolyte Fuel Cells," Journal of the Electrochemical Society, 140: 5 (May), 1218-1225.
- Gallopoulos, E., Houstis, E. & Rice, J.R.(1994), "Computer as Thinker/Doer: Problem-Solving Environments for Computational Science," IEE Computational Science & Engineering 1070-9924/94 (Summer), 1-23.
- He, W. (1994a), "A Simulation Model for Integrated Molten Carbonate Fuel Cell Systems," Journal of Power Sources, 49, 283-290.

- He, W. (1994b), "The Dynamic Performance of a Molten Carbonate Fuel Cell in Power-Generation Systems," *Journal of Power Sources*, 52, 179-184.
- Keon, N., Simader, G., Ören, T.I., Oliveira, J.C.T. (1995), "Modeling and Simulation of the Proton Exchange Membrane Fuel Cell: A State of the Art Review," *Proceedings of the 1995 Summer Computer Simulation Conference*, The Society for Computer simulation, San Diego, CA, 659-664.
- Koene, F.G.H., Mallant, R. & Ruiter, T. (1993), "Report of the ECN Activities in the IEA PEFC Group," Netherlands Energy Research Foundation.
- Kordesch, K.V. & Oliveira, J.T. (1985), "Fuel Cells," *Ullman's Encyclopedia of Industrial Chemistry*, Fifth edition, VCH, Weinheim, Germany, Vol. A 12, pp.55-83.
- Kordesch, K.V. & Simader, G.R. (1995), "Environmental Impact of Fuel Cell Technology," *Chemical Reviews*, 95: 1, 191-207.
- Lowry, M.R. (1991), "Software Engineering in the Twenty-First Century," *Conclusion, Automating Software Design*, AAAI Press/The MIT Press, London, 627-654.
- Nguyen, T.V. & White, R.E. (1993), "A Water and Heat Management Model for Proton-Exchange-Membrane Fuel Cells," *Journal of the Electrochemical Society*, 140: 8 (August), 2178-2186.
- Ören, T.I. (1984), "GEST - A Modelling and Simulation Language Based on System Theoretic Concepts," *NATO ASI Series, Vol. F10, Simulation and Model-Based Methodologies: An Integrative View*, Springer-Verlag, Berlin Heidelberg, 281-334.
- Ören, T.I. (1994), "Artificial Intelligence in Simulation," *Annals of Operations Research*, 53, 287-319.
- Ören, T.I. & Ghasem-Aghaee, N. (1995), "Front-End Interfaces for Simulation Environments: Quality Criteria and Visual Basic®'s Event-Based Approach," *University of Ottawa, Technical Report, TR 95-02*.
- Qiang, J. (1993), "SimGest: A Simulation Experimentation Environment and a Program Generator for Interactive Simulation," *University of Ottawa, Thesis (M.Sc. Systems Science)*.
- Segal, B.G. (1985), "Chemical Kinetics", chapter 19, *Chemistry: Experiment and Theory*, John Wiley & Sons, Inc., Toronto, Ontario, pp.707-744.

Springer, T.E., Wilson, M.S., & Gottesfeld, S. (1993), "Modeling and Experimental Diagnostics in Polymer Electrolyte Fuel Cells," *Journal of the Electrochemical Society*, 140. 12 (Dec.), 3513-3526.

Springer, T.E., Zawodzinski, T.A. & Gottesfeld, S. (1991), "Polymer Electrolyte Fuel Cell Model," *Journal of the Electrochemical Society*, 138: 8 (Aug.), 2334-2342.

Stanislav, J.F. (1982), *Mathematical Modelling of Transport Phenomena Processes*, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Wymore, A.W. (1967), *A Mathematical Theory of Systems Engineering*, Wiley, New York.

## **Appendices: An Example Problem**

This appendices contains the dynamic model of a proton exchange membrane fuel cell, used to generate the graphs in Section 5.4. Of further interest to the reader, the model is presented as a comparison of the same simulation run in ACSL and GestCell.

The model is first presented in appendix A in GestCell, with some sample output. Subsequently, in appendix B the model is presented in ACSL, including similar graphs as in section 5.4 and some sample output. The variable names have slight variations between the implementations, but the model equations are identical. It is hoped that the following sections will provide an example of how the GestCell system provides a powerful presentation of a model, in contrast to a traditional simulation language.

## Appendix A: PEMFC Model and Simulation in GestCell

### Gest specification of the PEMFC model:

GEST Specification						
name	description	value	units	lower limit	upper limit	
<b>Continuous Model</b>						
PEMFC	Continuous GEST Model of a PEMFC					
<b>Model declarations</b>						
<b>Independent variable</b>						
t	time		s	0		
<b>Input variables</b>						
i	current density		A/π <sup>2</sup>	0	1.5	
<b>State variables</b>						
default initial values						
Hg	density of hydrogen gas in the anode feedstream	1.035274E-01	mol/L	0		
OXg	density of oxygen in the cathode feedstream	8.282189E-02	mol/L	0		
Wg	density of water vapour in the cathode feedstream	2.070547E-02	mol/L	0		
<b>Auxiliary variables</b>						
D	diffusion coefficient of the electrodes (Koene et al. use a value, E1, which seems to be typo for Er, for which I have used VOLTo)			0		
Fain	total gas feed rate to the anode feedstream		mol/s	0		
FAout	total gases removed from the anode feedstream		mol/s	0		
Fcin	total gass feed rate to the cathode feedstream		mol/s	0		
FCout	total gases removed from the cathode feedstream		mol/s	0		
feedHg	feed rate of hydrogen gas to the anode		mol/s	0		
feedOXg	feed rate of oxygen gas to the cathode feedstream		mol/s	0		

feedWc	feed rate of water vapour to the cathode feedstream	mol/s	0
HgOut	pressure is regulated	mol/s	
hHg	enthalpy of hydrogen gas in the anode feedstream	kJ/mol	
hOXg	enthalpy of oxygen gas in the cathode feedstream	kJ/mol	
hTot	overall rate of heat production - heat of formation of water for simplicity	kJ/s	
hWg	enthalpy of water vapour in the cathode feedstream	kJ/mol	
ixch	exchange current density used in POLact	A/m <sup>2</sup>	0
Na	moles of gas in the anode feedstream	mol	0
Nc	moles of gas in the cathode feedstream	mol	0
Nda	desired no. of moles in the anode feedstream to maintain system at desired pressure	mol	0
Ndc	desired no. of moles in the cathode feedstream to maintain the system at the desired pressure	mol	0
Nemst	voltage given by Nemst equation - pressure dependency	V	
NHga	mols of hydrogen gas in the anode feedstream	mol	0
NOXc	moles of oxygen gas in the cathode feedstream	mol	0
NWc	moles of water vapour in the cathode feedstream	mol	0
OXgOut	pressure is regulated	mol/s	
Pdens	power density	(V*i)/m <sup>2</sup>	
PHg	partial pressure of hydrogen gas in the anode feedstream	atm	0
POLact	activation polarization	V	0
POLconc	concentration polarization - combination of Fick's law with Nemst's law	V	0
POLohm	ohmic polarization in the cell	V	0
POLthem	all energy that is not electrical energy or polarization is assumed lost to cooling		
POXg	partial pressure of oxygen in the cathode feedstream	atm	0
PWg	partial pressure of water vapour in the cathode feedstream	atm	0
areaRes	area resistance of the fuel cell	ohm*(m <sup>2</sup> )	0
rate	overall rate of reaction in the fuel cell rate of production of H2O	mol/s	0
Volt	output voltage of the fuel cell	V	
WgOut	pressure is regulated	mol/s	

Constants					
Avog	Avogadro's constant	6.022045E+23	atm		
Boltz	Boltzmann's constant	1.380662E-23	V		
e	elementary charge on 1 electron	1.602089E-19			
Faraday	Faraday constant	9.648500E+04	C/mol		
mH	molar mass of Hydrogen	2.016000E+00	2.0		
mOX	molar mass of Oxygen	1.801700E+01	g/mol		
mW	molar mass of water	3.199800E+01	g/mol		
R1	first gas constant - depends on units	8.206000E-02	(L*atm) / (mol*K)		
R2	second gas constant - depends on units	8.314410E+00	J/(mol*K)		
stdhHg	standard enthalpy of formation of hydrogen gas (298 K)	0.000000E+00	kJ/mol		
stdhOXg	standard enthalpy of formation of oxygen gas (298 K)	0.000000E+00	kJ/mol		
stdWg	standard enthalpy of formation of water vapour (298 K)	-2.418300E+02	kJ/mol		
VOLTo	standard theoretical voltage for PEMFC	1.229000E+00	V		
Parameters		default values			
alpha	transfer coefficient - used in calculation of activation polarization	5.000000E-01			
Area	surface area of the fuel cell electrodes	1.000000E+00	m <sup>2</sup>	0	
CpCell	heat capacity of the fuel cell structure	8.500000E-01	kJ/(g*K)	0	
CpHg	heat capacity of hydrogen gas	8.150000E-04	atm	0	
CpOXg	heat capacity of oxygen gas	5.234000E-05	atm	0	
CpW	heat capacity of water vapour	2.390050E-01	atm	0	
de	thickness of the electrolyte	1.000000E-04	m	0	
Do	standard diffusion coefficient value - D, the diffusion coefficient, exhibits Arrhenius behaviour	0.00000018		0	
Eact	fundamental activation energy of the overall electrochemical reaction	6.600000E-01	A/m <sup>2</sup>		
Ei	value used in calculation of diffusion coefficient	1.400000E-01	eV		
MemPartDens	particle density of the electrolyte membrane	2.110600E+24	1/m <sup>3</sup>	0	
hgfa	mole fraction of hydrogen fed to the anode feedstream	1.000000E+00		0	1
ilim	limiting current density of the fuel cell	1.000000E+04	A/m <sup>2</sup>	0	
K	reaction rate coefficient	2.000000E+07		0	
mass	mass of the fuel cell structure	5.000000E+03	g		
n	number of electrons involved in overall cell reaction	2.000000E+00			
oxfc	mole fraction of oxygen gas fed to the cathode feedstream	8.000000E-01		0	1

Pad	desired pressure in the anode feedstream - pressure is regulated	3.000000E+00	atm	0	
Pcd	desired pressure in the cathode feedstream - pressure is regulated	3.000000E+00	atm	0	
res	internal resistance of the fuel cell	5.000000E-01	ohm	0	
stoicHg	stoichiometric coefficient for hydrogen gas in the anode	1.000000E+00			
stoicOXg	stoichiometric coefficient for oxygen gas in the cathode	5.000000E-01			
stoicW	stoichiometric coefficient for water in the cathode	1.000000E+00			
Ta	Temperature of the anode feedstream	3.531300E+02	K	0	
Tc	temperature in the cathode feedstream	3.531300E+02	K	0	
Tfc	temperature of the fuel cell structure	3.531300E+02	K	0	
trcoeff	transfer coefficient, in POLact	5.000000E-01			
Va	volume of the anode feedstream	1.000000E+00	L		
Vc	volume of the cathode feedstream	1.000000E+00	L		
wgfa	mole fraction of water vapour fed to the anode feedstream	0.000000E+00		0	1
wgfc	mole fraction of water vapour fed to the cathode feedstream	2.000000E-01		0	1

#### Dynamic

##### Input functions

i = 5000 A/m<sup>2</sup> 0 1.5

##### Auxiliary variables

D	= Do*exp(-Ei / (K*Tfc))			0	
Fain	= feedHg		mol/s	0	
FAout	= HgOut		mol/s	0	
Fcin	= feedOXg + feedWc		mol/s	0	
FCout	= OXgOut + WgOut		mol/s	0	
feedHg	= (rate/0.8)		mol/s	0	
feedOXg	= (rate/0.5)		mol/s	0	
feedWc	= (wgfc/oxfc)*feedOXg		mol/s	0	
HgOut	= (NHga/Na)*(Na-Nda)		mol/s		
hHg	= stdhHg		kJ/mol		
hOXg	= stdhOXg		kJ/mol		
hTot	= (hWg - hOXg - hHg)*rate		kJ/s		
hWg	= stdWg		kJ/mol		
iexch	= K*exp(Eact / (K*Tfc))		A/m <sup>2</sup>	0	
Na	= NHga		mol	0	
Nc	= NOXc + NWc		mol	0	
Nda	= (Pad*Va) / (R1*Ta)		mol	0	
Ndc	= (Pcd*Vc) / (R1*Tc)		mol	0	
Nemst	= VOLTo + (((R2*Tfc)/(n*Faraday)) * (log(PHg/PWg) + log(0.5/POXg)))		V		
NHga	= Hg*Va		mol	0	
NOXc	= OXg*Vc		mol	0	
NWc	= Wg*Vc		mol	0	
OXgOut	= (NOXc/Nc)*(Nc-Ndc)		mol/s		
Pdens	= Volt*i		(V*i)/m <sup>2</sup>		
PHg	= (NHga*R1*Ta)/Va		atm	0	

POLact	= ((Boltz*Tfc) / (2*e*alpha)) * (log(i/iexh))	V	0
POLconc	= ((Boltz*Tfc) / (2*e)) * (log(1-(i/ilm)))	V	0
POLOhm	= i*areaRes	V	0
POLtherm	= -hTot - (Pdens*Area/1000)		
POXg	= (NOXc*R1*Tc)/Vc	atm	0
PWg	= (NWc*R1*Tc)/Vc	atm	0
areaRes	= ((de*Boltz*Tfc) / (D*(pow(e,2))*MemPartDens))	ohm*(m^2)	0
rate	= (i*Area) / (2*Faraday)	mol/s	0
Volt	= Nernst - POLohm + POLact + POLconc	V	
WgOut	= (NWc/Nc)*(Nc - Ndc)	mol/s	
<b>Derivatives</b>			
Hg'	= (feedHg - HgOut - (stoicHg*rate))/Va	mol/(L*s)	0
OXg'	= (feedOXg - OXgOut - (stoicOXg*rate))/Vc	mol/(L*s)	0
Wg'	= (feedWc - WgOut + (stoicW*rate))/Vc	mol/(L*s)	0

**End Model**

**Parameter Set 1**

	default set			
alpha	transfer coefficient - used in calculation of activation polarization	5.000000E-01		
Area	surface area of the fuel cell electrodes	1.000000E+00	m^2	0
CpCell	heat capacity of the fuel cell structure	8.500000E-01	kJ/(g*K)	0
CpHg	heat capacity of hydrogen gas	8.150000E-04	atm	0
CpOXg	heat capacity of oxygen gas	5.234000E-05	atm	0
CpW	heat capacity of water vapour	2.390050E-01	atm	0
de	thickness of the electrolyte	1.000000E-04	m	0
Do	standard diffusion coefficient value - D, the diffusion coefficient, exhibits Arrhenius behaviour	0.00000018		0
Eact	fundamental activation energy of the overall electrochemical reaction	6.600000E-01	A/m^2	
EI	value used in calculation of diffusion coefficient	1.400000E-01	eV	
MemPartDens	particle density of the electrolyte membrane	2.110600E+24	1/m^3	0
hgfa	mole fraction of hydrogen fed to the anode feedstream	1.000000E+00		0 1
ilm	limiting current density of the fuel cell	1.000000E+04	A/m^2	0
K	reaction rate coefficient	2.000000E+07		0
mass	mass of the fuel cell structure	5.000000E+03	g	
n	number of electrons involved in overall cell reaction	2.000000E+00		
oxfc	mole fraction of oxygen gas fed to the cathode feedstream	8.000000E-01		0 1

Pad	desired pressure in the anode feedstream - pressure is regulated	3.000000E+00	atm	0	
Pcd	desired pressure in the cathode feedstream - pressure is regulated	3.000000E+00	atm	0	
res	internal resistance of the fuel cell	5.000000E-01	ohm	0	
stoicHg	stoichiometric coefficient for hydrogen gas in the anode	1.000000E+00			
stoicOXg	stoichiometric coefficient for oxygen gas in the cathode	5.000000E-01			
stoicW	stoichiometric coefficient for water in the cathode	1.000000E+00			
Ta	Temperature of the anode feedstream	3.531300E+02	K	0	
Tc	temperature in the cathode feedstream	3.531300E+02	K	0	
Tfc	temperature of the fuel cell structure	3.531300E+02	K	0	
trcoeff	transfer coefficient, in POLact	5.000000E-01			
Va	volume of the anode feedstream	1.000000E+00	L		
Vc	volume of the cathode feedstream	1.000000E+00	L		
wgfa	mole fraction of water vapour fed to the anode feedstream	0.000000E+00		0	1
wgfc	mole fraction of water vapour fed to the cathode feedstream	2.000000E-01		0	1
<b>End Parameter Set</b>					
<b>Initial Value Set 1</b>					
Hg	density of hydrogen gas in the anode feedstream	1.035274E-01	mol/L		
OXg	density of oxygen in the cathode feedstream	8.282189E-02	mol/L	0	
Wg	density of water vapour in the cathode feedstream	2.070547E-02	mol/L	0	
<b>End Initial Value Set 1</b>				0	
<b>Experiment 1</b>					
default experiment					
<b>Observe</b>					
Input variables					
i					
Output variables					
State variables					
Auxiliary variables					
POLohm					
POLconc					
POLact					
Volt					
PWg					
POXg					
PHg					
Nernst					
Observe at every	communication interval	1.000000E-01			
Integrate by	Runge-Kutta 4				
	integration step size	1.000000E-02			
Start at					
tinit	initial time	0.000000E+00			
Terminate when t >=					
tfinal	time condition	3.000000E+01	s		
<b>End Experiment 1</b>					

Top of Output from the Simulation Run:

Note: Run used current density,  $i = 500 \text{ A/m}^2$ , from an initial state of  $i = 0$

Parameter Set			1								
Initial Value Set			1								
Expenment			1								
Communication Interval			0.1								
Number of Points			301								
Point	t	i	Nernst	PHg	POLact	POLconc	POLohm	POXg	PWg	Voit	
0	0	5000	1.22962	3	-0.25241	-0.01055	0.25	2.4	0.6	0.716667	
1	0.11	5000	1.22622	3.01955	-0.25241	-0.01055	0.25	2.51358	0.721056	0.713266	
2	0.21	5000	1.22372	3.03556	-0.25241	-0.01055	0.25	2.60072	0.825939	0.710761	
3	0.31	5000	1.22163	3.05004	-0.25241	-0.01055	0.25	2.67471	0.925707	0.708672	
4	0.41	5000	1.21986	3.06314	-0.25241	-0.01055	0.25	2.73731	1.02032	0.706904	
5	0.51	5000	1.21835	3.07499	-0.25241	-0.01055	0.25	2.79004	1.10985	0.705393	
6	0.61	5000	1.21704	3.08572	-0.25241	-0.01055	0.25	2.8342	1.19441	0.70409	
7	0.71	5000	1.21591	3.09542	-0.25241	-0.01055	0.25	2.87091	1.27417	0.702958	
8	0.81	5000	1.21492	3.10421	-0.25241	-0.01055	0.25	2.90114	1.34933	0.70197	
9	0.91	5000	1.21406	3.11215	-0.25241	-0.01055	0.25	2.92572	1.4201	0.701103	
10	1.01	5000	1.21329	3.11934	-0.25241	-0.01055	0.25	2.94541	1.4867	0.700338	

## Appendix B:

### PEMFC Model and Simulation in ACSL

PROGRAM Model - PEMFC

!-----This model has 3 differential equations  
!-----describing mass balances in the cell

INITIAL

```

!-----Simulation Time
      CONSTANT Tstp=30.0      !s

!-----Pressure and Temp. taken as constant
      !-----taken from Springer, et. al.[1991], p.2338,table1
      CONSTANT Pad=3.0 , Pcd=3.0 !atm units
      CONSTANT Tc=353.15 !Kelvin - 80 Celsius
      CONSTANT Ta=353.15
      CONSTANT Tfc=353.15

!-----Parameters - used in calculation of Voltage
!-----voltage calculation base on Koene, et al. (1994)
      CONSTANT alpha = 0.5 !transfer coefficient - used in calculation of
      activation polarization
      CONSTANT Do = 0.00000018 !standard diffusion coefficient value - D, the
      diffusion coefficient, exhibits Arrhenius behaviour
      CONSTANT Eact = 0.66 !fundamental activation energy of the overall
      electrochemical reaction, A/m^2
      CONSTANT El = 0.14 !value used in calculation of diffusion
      coefficient, eV
      CONSTANT MPDns = 2.110600E+24 ! particle density of the electrolyte
      membrane, 1/m^3
      CONSTANT ilim = 1.000000E+04 !limiting current density of the fuel
      cell, A/m^2
      CONSTANT K = 2.000000E+07 !reaction rate coefficient
      CONSTANT n = 2.00 !number of electrons involved in overall cell
      reaction
      CONSTANT trcoeff = 0.5 !transfer coefficient, in POLact

!-----Parameters - properties of pemfc
      CONSTANT Area =1.0 !area of the fuel cell, m^2
      CONSTANT de = 0.0001 !distance across the electrolyte, m
      CONSTANT Va =1.0 ! GUESS - Volume, L
      CONSTANT Vc =1.0 ! GUESS - Volume, L
      CONSTANT mass=5000.0 !MASS of the fuel cell, g
      CONSTANT CpCell=0.85 !heat capacity of the cell, kJ/g*K

!-----Parameters - gases and reactions

```

```

CONSTANT stHg=1.0      !Stoichiometric coefficient for hydrogen at the
  anode
CONSTANT stOXg=0.5    !Stoichiometric coefficient for oxygen at the
  cathode
CONSTANT stW=1.0      !Stoichiometric coefficient for water in the cell
CONSTANT hgfa=1.0     !feed rate of hydrogen gas to fuel cell
CONSTANT oxfc=0.8     !feed rate of oxygen gas to fuel cell
CONSTANT wgfa=0.0     !feed rate of water vapour to fuel cell (anode)
CONSTANT wgfc=0.2     !feed rate of water vapour to fuel cell (cathode)

```

```

!-----heat capacities & fundamental enthalpies
!-----taken from CRC handbook

```

```

CONSTANT CpHg = 0.000815      !25 deg Celsius, kJ/g*K
CONSTANT CpOXg = 0.00005234   !25 deg Celsius, kJ/g*K
CONSTANT CpW = 0.239005      !100 deg Celsius, kJ/g*K
CONSTANT sthHg = 0.0          ! kJ/mol
CONSTANT sthOXg = 0.0         ! kJ/mol
CONSTANT stdWg = -241.83      ! kJ/mol

```

```

!-----Constants

```

```

CONSTANT mH = 2.016      !Molar mass of H2, g/mol
CONSTANT mOX = 18.017   !Molar mass of O2, g/mol
CONSTANT mW = 31.998    !Molar mass of H2O, g/mol
!THE FARADAY CONSTANT & AND GAS CONSTANT

```

```

CONSTANT R1 = 8.206000E-02 !first gas constant - depends on units,
  (L*atm) / (mol*K)
CONSTANT R2 = 8.314410E+00 !second gas constant - depends on units,
  J/(mol*K)
CONSTANT Farad = 96485.0    ! CHARGE ON 1MOL OF e-'s, C/mol
CONSTANT Avog = 6.022045E23 ! Avogadro's number, 1/mol
CONSTANT Boltz = 1.380662E-23 !Boltzmann's constant, V
CONSTANT e = 1.602089E-19  !elementary charge on 1 electron
CONSTANT VOLTo = 1.229000E+00 !standard theoretical voltage for PEMFC, V

```

```

!-----Initial Values

```

```

!-----Anode feedstream

```

```

Hgi = 1.035274E-01      !density of hydrogen gas in the anode
  feedstream, mol/L

```

```

!-----Cathode Feedstream

```

```

!ASSUME 80%O2 - 20%H2O MIXTURE (at 3 atm)

```

```

OXgi = 8.282189E-02     !density of oxygen in the cathode
  feedstream, mol/L

```

```

Wgi = 2.070547E-02     !density of water vapour in the cathode
  feedstream, mol/L

```

```

END      !of initial

```

```

DYNAMIC

```

DERIVATIVE

```

!-----Integration Algorithm and Step Size
ALGORITHM Ialg = 5
MAXTERVAL Maxt = 0.01
NSTEPS Nstp = 1
!-----Communication Interval
CINTERVAL Cint = 0.1

!-----Current density set outside the cell
i = 5000.0 !current density, A/m^2

!-----convert current to units in model

rate = (i*Area) / (2*Farad) ! converts desired current from
! amps/m^2 to mol/s
! for overall reaction rate in the cell

!-----Moles of gas in particular regions at any time
!-----Note: No gas in PEM - only protons and liquid water
NHga = Hg*Va !ANODE FEEDSTREAM, mol
Na = NHga !mol
NOXc = OXg*Vc !CATH. FEEDSTREAM, mol
NWc = Wg*Vc ! mol
Nc = NOXc + NWc !mol
!-----Desired no. of moles of gas to keep press. and temp. constant
Nda = (Pad*Va) / (R1*Ta) ! mol
Ndc = (Pcd*Vc) / (R1*Tc) ! mol

!-----Calculate partial pressures
PHg = (NHga*R1*Ta)/Va !atm
POXg = (NOXc*R1*Tc)/Vc !atm
PWg = (NWc*R1*Tc)/Vc !atm

!-----Input and Output rules for the feedstreams
!-----in order to keep pressure constant - trick for ISOBARIC
!-----Input rules
!rate of gases fed to feedstreams
fdHg = (rate/0.8) !mol/s
fdOXg = (rate/0.5) !mol/s
fdWc = (wgfc/oxfc)*fdOXg ! H2O fed to cathode, mol/s

!-----Total gas flow into feedstreams
Fain = fdHg ! mol/s
Fcin = fdOXg + fdWc ! mol/s

!-----Output rules
!-----assumes well-mixed gases - ie. constant ratios of gases
! throughout the feedstream and gases leave in
! the same ratio as they are present
! output of gases determined by
! desired pressure in the feedstream, ie. 3 atm

```

```

HgOut = (NHga/Na)*(Na-Nda)                                ! mol/s
      ! H2 let out of the anode feedstream (only gas present)
OXgOut = (NOXc/Nc)*(Nc-Ndc)                                ! mol/s
      ! O2 let out of the cathode feedstream
WgOut = (Nwc/Nc)*(Nc - Ndc)                                ! mol/s
      ! W let out of the cathode feedstream

      !-----Total gas flow out of feedstreams
FAout = HgOut                                             ! mol/s
FCout = OXgOut + WgOut                                     ! mol/s

      !-----Enthalpies of the gases in the feedstreams
hHg = sthHg                                               !kJ/mol
hOXg = sthOXg                                             !kJ/mol
hWg = stdWg                                               !kJ/mol

      !-----rate of Overall Heat released by reaction, ie. change in
      enthalpy

hTot = (hWg - hOXg - hHg)*rate                            !kJ/s

!Ignore heat flux - ASSUME all energy other than electrical output
!is THERMAL LOSSES
POLth = -hTot - (Pdens*Area/1000)

      !-----Calculate the voltage
      !-----assuming activities are unity
      !VOLTo = 1.229 ! STANDARD VALUE, V
      !n = 2.0      ! # of e-'s in reaction
      !FARAD = 96485.0      ! CHARGE ON 1MOL OF e-'s, C/mol
Nernst = VOLTo + (((R2*Tfc)/(n*Farad)) * &
      (log(PHg/PWg) + log(0.5/POXg)))      ! V

      !-----polarization losses (Koene, et al.)
      !-----check these functions with Guenter
D = Do*exp(-E1 / (K*Tfc))
areaRs = ((de*Boltz*Tfc) / (D*(e**2)*MPDns))      ! ohm*(m^2)
POLohm = i*areaRs      ! V

!
      K = 2.0      ! rate constant
      BOLTZ = 1.380662E-23
      alpha = 0.5

iexch = K*exp(Eact / (K*Tfc))      !A/m^2
POLact = ((Boltz*Tfc) / (2*e*alpha)) * (log(i/iexch))      !V

POLcon = ((Boltz*Tfc) / (2*e)) * (log(1-(i/ilim)))      !V

      !-----Power Density

```

```

Volt = Nernst - POLohm + POLact + POLcon      !V
Pdens = Volt*i      !(V*i)/m^2

!-----Dynamic Equations
!-----???d denotes differential equation

!-----Anode Feedstream
! mass of H2 in anode feedstream
Hgd = (fdHg - HgOut - (stHg*rate))/Va      !mol/L*s
!-----Cathode Feedstream
! mass of O2 in cathode feedstream
OXgd = (fdOXg - OXgOut - (stOXg*rate))/Vc  !mol/L*s
! mass of H2O in cathode feedstream
Wgd = (fdWc - WgOut + (stW*rate))/Vc      !mol/L*s

!-----Integrate differential equations

!-----Anode Feedstream
Hg = INTEG(Hgd, Hgi)

!-----Cathode Feedstream
OXg = INTEG(OXgd, OXgi)
Wg = INTEG(Wgd, Wgi)

END !of Derivative

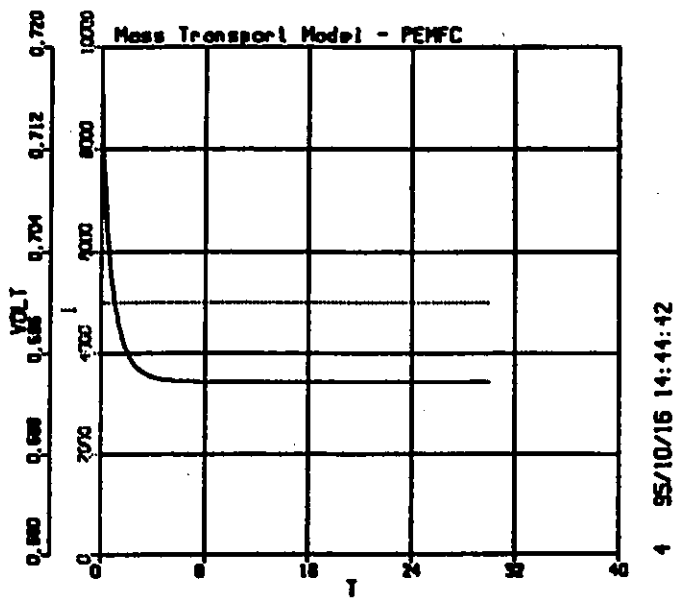
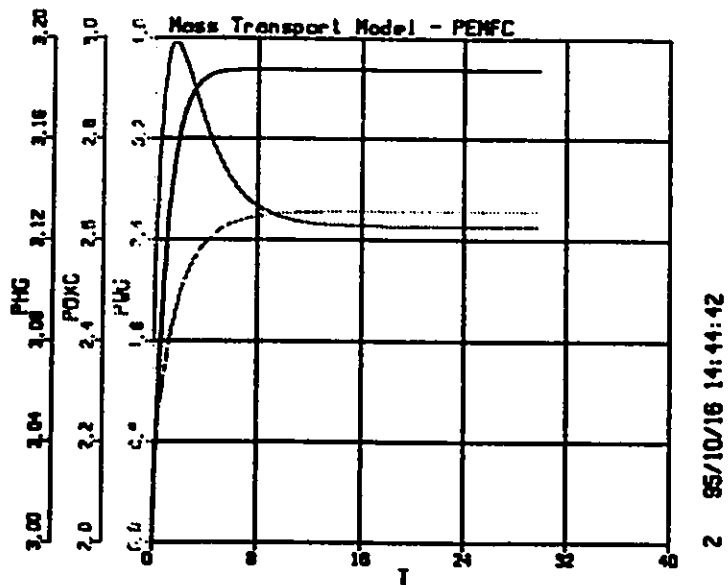
!-----Termination Condition
TERMT(T .GE. Tstp)

END !of Dynamic

END ! of Program

```

Graphs from ACSL Run:



Top of Output from ACSL Run:

T 0. POLACT-0.25242200 PHG 3.00017000 I 5000.00000	VOLT 0.71663700 POLCON-0.01054760 POXG 2.40014000	NERNST 1.22962000 POLOHM 0.25001400 PWG 0.60003400
T 0.10000000 POLACT-0.25242200 PHG 3.01802000 I 5000.00000	VOLT 0.71351400 POLCON-0.01054760 POXG 2.50419000	NERNST 1.22650000 POLOHM 0.25001400 PWG 0.71032900
T 0.20000000 POLACT-0.25242200 PHG 3.03417000 I 5000.00000	VOLT 0.71096100 POLCON-0.01054760 POXG 2.59275000	NERNST 1.22394000 POLOHM 0.25001400 PWG 0.81571900
T 0.30000000 POLACT-0.25242200 PHG 3.04878000 I 5000.00000	VOLT 0.70883500 POLCON-0.01054760 POXG 2.66797000	NERNST 1.22182000 POLOHM 0.25001400 PWG 0.91600400
T 0.40000000 POLACT-0.25242200 PHG 3.06200000 I 5000.00000	VOLT 0.70703800 POLCON-0.01054760 POXG 2.73163000	NERNST 1.22002000 POLOHM 0.25001400 PWG 1.01114000
T 0.50000000 POLACT-0.25242200 PHG 3.07397000 I 5000.00000	VOLT 0.70550400 POLCON-0.01054760 POXG 2.78528000	NERNST 1.21849000 POLOHM 0.25001400 PWG 1.10117000
T 0.60000000 POLACT-0.25242200 PHG 3.08479000 I 5000.00000	VOLT 0.70418100 POLCON-0.01054760 POXG 2.83024000	NERNST 1.21717000 POLOHM 0.25001400 PWG 1.18622000
T 0.70000000 POLACT-0.25242200 PHG 3.09459000 I 5000.00000	VOLT 0.70303400 POLCON-0.01054760 POXG 2.86765000	NERNST 1.21602000 POLOHM 0.25001400 PWG 1.26645000
T 0.80000000 POLACT-0.25242200 PHG 3.10345000 I 5000.00000	VOLT 0.70203200 POLCON-0.01054760 POXG 2.89848000	NERNST 1.21502000 POLOHM 0.25001400 PWG 1.34206000
T 0.90000000 POLACT-0.25242200 PHG 3.11147000 I 5000.00000	VOLT 0.70115400 POLCON-0.01054760 POXG 2.92359000	NERNST 1.21414000 POLOHM 0.25001400 PWG 1.41327000

T 1.00000000  
POLACT-0.25242200  
PHG 3.11872000  
I 5000.00000

VOLT 0.70038000  
POLCON-0.01054760  
POXG 2.94373000

NERNST 1.21336000  
POLOHM 0.25001400  
PWG 1.48027000