DECLARATIVE MODELING OF PROTON EXCHANGE MEMBRANE FUEL CELLS FOR SYSTEM DESIGN

A Dissertation
Presented to
The Academic Faculty

by

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LISTS OF ABBREVIATIONS

Acronyms

CFD	Computational fluid dynamics
EOS	Equation of state
GDL	Gas diffusion layer
ISO	International Standards Organization
MEA	Membrane electrode assembly
PEM	Proton exchange (or polymer electrolyte) membrane
PEMFC	Proton exchange (or polymer electrolyte) membrane fuel cell
SSSF	Steady state, steady flow (noun or adjective)

Electrochemical Components

e^-	Electrons
H^+	Protons
H_2	Diatomic hydrogen
H_2O	Water
N_2	Diatomic nitrogen
O_2	Diatomic oxygen
Pt^+	Platinum ions (charge number +1)
SO_3^-	Sulfonic acid

NOMENCLATURE[i] [ii]

Symbols

A	Area $[\mathrm{L}^2]$
a	Thermodynamic activity $[1]$ or gravitational acceleration $[\mathrm{L}\,\mathrm{T}^{-2}]$
b	Correlation coefficient [misc.]
C	Heat capacity [N]
c	Specific heat capacity [1]
D	Hydraulic diameter [L] or self diffusivity $[\mathrm{L}^2\,\mathrm{T}^{-1}]$
d	Specific particle diameter $[\mathrm{L}\,\mathrm{N}^{-1}]$
E	Electric field $[\mathrm{L}\,\mathrm{M}\,\mathrm{N}^{-1}\,\mathrm{T}^{-2}]$
f	Force $[\mathrm{L}\,\mathrm{M}\,\mathrm{T}^{-2}]$
g	Specific Gibbs energy $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{N}^{-1}\,\mathrm{T}^{-2}]$
H	Enthalpy $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{T}^{-2}]$
h	Specific enthalpy $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{N}^{-1}\,\mathrm{T}^{-2}]$ or heat transfer coefficient $[\mathrm{N}\,\mathrm{L}^{-2}\,\mathrm{T}^{-1}]$
I	Material current $[\mathrm{N}\,\mathrm{T}^{-1}]$
i	Integer index [–]
J	Generic flux $[\text{misc.} \times \mathrm{L}^{-2}]$
j	Integer index [–]
k	General constant or correlation coefficient [misc.]
Kn	Knudsen number [1]
L	Length [L]
M	Mass [M]
m	Specific mass $[\mathrm{M}\,\mathrm{N}^{-1}]$ or cardinality [–]
$m\Phi$	Linear momentum $[\mathrm{L}\,\mathrm{M}\,\mathrm{T}^{-1}]$
N	Particle number [N]
n	Integer number (e.g., stoichiometric coefficient) [–]
Nu	Nusselt number [1]
P	Perimeter [L]
p	Pressure $[\mathrm{M}\,\mathrm{L}^{-1}\,\mathrm{T}^{-2}]$
Pe	Péclet number [1]
Q	Heat $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{T}^{-2}]$
q	Single particle [N]
R	Generalized resistance [misc.] or electrical resistance $[\mathrm{M}\,\mathrm{L}^2\,\mathrm{T}^{-3}]$
r	Generalized resistivity [misc.]
Re	Reynolds number [1]
S	Entropy [N]
s	Specific entropy [1]
T	Temperature $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{N}^{-1}\,\mathrm{T}^{-2}]$
t	Time [T]
U	Internal energy $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{T}^{-2}]$

[i] The dimensions are noted in terms of angle (A), length (L), mass (M), particle number (N), and time (T). See Section **??** for details.

[ii] Although not shown here, boldface is used to denote vector quantities and operations.

V	Volume $[\mathrm{L}^3]$
v	Specific volume $[\mathrm{L}^3\,\mathrm{N}^{-1}]$ or electrical potential $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{N}^{-1}\,\mathrm{T}^{-2}]$
X	Generic conserved quantity [misc.]
x	Position along the x axis or generic axis of transport [L]
z	Position along the z axis [L] or charge number [1]
α	Adjusted collision interval [T] or charge transfer coefficient [1]
β	Dynamic compressibility $[\mathrm{N}\,\mathrm{T}\,\mathrm{L}^{-2}\,\mathrm{M}^{-1}]$
γ	Generic driving property for exchange or transport [misc.]
ε	Porosity [1] or permittivity $[\mathrm{N}^2\,\mathrm{T}^2\,\mathrm{L}^{-3}\,\mathrm{M}^{-1}]$
ϵ	Areic electrical capacitance $[\mathrm{N}^2\,\mathrm{T}^2\,\mathrm{L}^{-4}\,\mathrm{M}^{-1}]$
ζ	Fluidity $[\mathrm{L}\,\mathrm{T}\,\mathrm{M}^{-1}]$
η	Self resistivity $[\mathrm{T}\,\mathrm{L}^{-2}]$
θ	Thermal resistivity $[\mathrm{L}\,\mathrm{T}\,\mathrm{N}^{-1}]$
λ	Mean free path [L]
μ	Mobility $[\mathrm{N}\,\mathrm{T}\,\mathrm{M}^{-1}]$ or dynamic viscosity $[\mathrm{M}\,\mathrm{L}^{-1}\,\mathrm{T}^{-1}]$
ν	Thermal independity [1]
ρ	Volumic particle number (i.e., density) $[\mathrm{N}\,\mathrm{L}^{-3}]$
τ	Time constant [T] or mean collision interval [T]
Φ	Product of particle number and velocity $[\mathrm{L}\,\mathrm{N}\,\mathrm{T}^{-1}]$
ϕ	Linear velocity $[\mathrm{L}\,\mathrm{T}^{-1}]$
ω	Flow diversion angle [A]

Accents

$\dot{}$	Flow rate of _ $[\times\mathrm{T}^{-1}]$

Superscripts

^{o}	_ at reference state
$^{\prime}$	Modified, effective, or characteristic _
*	Dimensionless _ [×misc.]

Subscripts

$_{1,\,2,\,3\,\text{or}\,\ldots}$	First, second, third or . . . _
$_{\mathrm{A}}$	_ of advection or advective
$_{\mathrm{a,\,b,\,c\,or\,\ldots}}$	First, second, third or . . . _
$_{\mathrm{c}}$	_ as, of, or in the condensed phase
$_{\mathrm{D}}$	_ of diffusion or diffusive
$_{\mathrm{DOF}}$	_ of degrees of freedom
$_{\mathrm{E}}$	_ of exchange
$_{\mathrm{g}}$	_ as, of, or in gas
$_{\mathrm{gen}}$	_ of generation
$_{\mathrm{i}}$	_ as, of, or in ionomer
$_{i}$	_ of index i
$_{\mathrm{IG}}$	_ of ideal gas
$_{j}$	_ of index j
$_{k}$	_ of index k

l	_ as, of, or in liquid
M	_ in the majority region
m	_ in the minority region
N	Material _
n	_ at or into the negative boundary
p	Isobaric _
phases	_ of phases
p	_ at or into the positive boundary
Q	Thermal _
sat	_ at saturation
spec	Set or _ of species in the region or in the chemical reaction
T	Isothermal _
T	_ of transport
tot	Total _
v	Isochoric _
x	_ along the x axis (through the cell)
y	_ along the y axis (down the channel)
z	_ along the z axis (across the channel)
ζ	_ for fluidity
θ	_ for thermal resistivity
Φ	Translational _
$\perp$	_ perpendicular to the axis of transport
$\parallel$	_ parallel to the axis of transport

GLOSSARY

configuration A species in a certain phase within a region 4

conversion property Effective intensive property of the sources in advective exchange . . 19

conversion temperature Entropy-weighted average temperature of the sources in advective thermal exchange $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{N}\,\mathrm{T}^{-2}]$ 27

conversion velocity Mass-weighted average velocity of the sources in advective translational exchange $[\mathrm{L}\,\mathrm{T}^{-1}]$ 26

dynamic compressibility Extent to which a non-equilibrium normal force causes or requires transient compression $[\mathrm{N}\,\mathrm{T}\,\mathrm{L}^{-2}\,\mathrm{M}^{-1}]$ 42

exchange Transfer of a conserved quantity among configurations within a region 16

independence Generalized resistance to diffusive exchange . . . . . x, 28

independity Specific independence 28

irreversible advection Transfer of a quantity due to material flow projected across the difference in a driving property between an interface and the upstream region or configuration 40

material current Flow rate of material $[\mathrm{N}\,\mathrm{T}^{-1}]$ 56

mediation property Conductance-weighted average property of configurations that interact within a region 20

mediation temperature Conductance-weighted average temperature of configurations that interact by thermal diffusion $[\mathrm{L}^2\,\mathrm{M}\,\mathrm{N}\,\mathrm{T}^{-2}]$ 28

mediation velocity Conductance-weighted average velocity of configurations that interact by translational diffusion $[\mathrm{L}\,\mathrm{T}^{-1}]$ 27

specific Adjective that indicates the quotient of the following quantity and its associated particle number $[\times\mathrm{N}^{-1}]$ . . . . . x, 3

translational Nusselt number Correction factor in the shear force equation (**??**) or Newton's law of viscous shear for the shape of the flow profile $[1]$ 46

transport Transfer of a conserved quantity between adjacent regions 30

CHAPTER 1

INTRODUCTION

> "The functionality and usefulness of computational fuel cell models in a design environment will require the effective and robust integration of the various submodels in a [computational fuel cell engineering] framework [...]. This will necessitate the development of novel algorithms that take into account the specific nature of the couplings, the large range of scales encountered in PEMFCs fuel cells (sic), and the multi-variable nature of the optimization problems."
>
> N. DJILALI [**?**]

1.1 Context and Motivation

Fuel cells (FCs) have the potential to serve a key role in our electric power networks, transportation systems, and portable electronic devices. In general FCs can convert fuel energy to work more efficiently and quietly than internal combustion engines (ICEs) [61], and a FC system's energy-to-power ratio can be easily adapted, unlike batteries. A FC system can be refueled quickly like an ICE system, or it can be designed to recharge like a battery by operating in electrolysis mode [**?**]. Of the various fuel cell technologies, proton exchange membrane fuel cells (PEMFCs) are best suited to meet the packaging and power-cycling requirements of vehicles and portable devices.

PEMFCs have a solid polymer-based electrolyte and operate at low temperatures (typically below 100 $^{\circ}$C). As shown in Figure 1.1, a single-cell PEMFC has few core components: proton exchange membrane (PEM), catalyst layers (CLs) or electrodes, gas diffusion layers (GDLs), and flow plates (FPs) [61]. However, most applications require a higher voltage than a single-cell PEMFC can provide; therefore, two or more cells are joined back-to-back to form a PEMFC stack like the one shown in Figure 1.2.

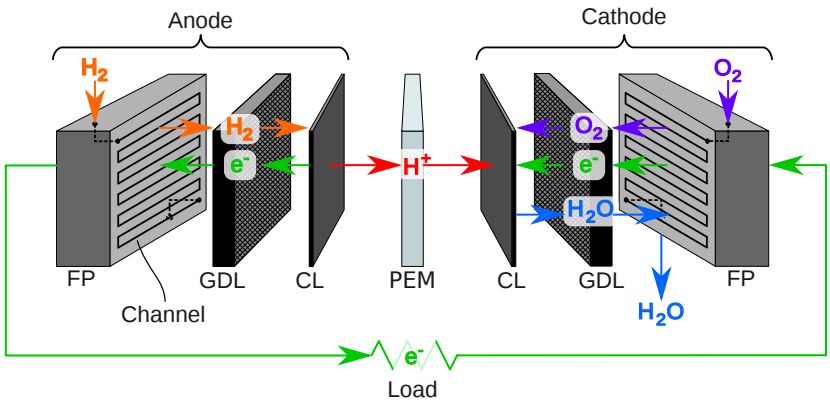


Figure 1.1: Layers of a single-cell PEMFC and the primary paths of electrons (e^-), protons (H^+), hydrogen (H_2), oxygen (O_2), and water (H_2O) during normal operation..

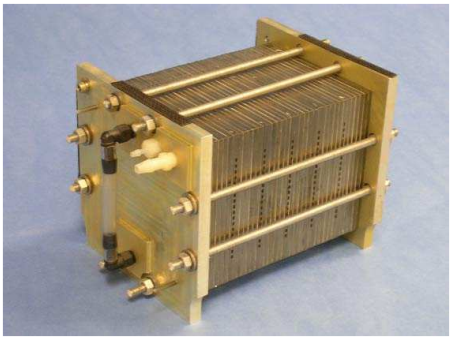


Figure 1.2: 500 W, 32-cell, water-cooled PEMFC used to power an unmanned aerial vehicle [**?**]..

A PEMFC operates on the chemical energy released by the reaction of hydrogen (H_2) and oxygen (O_2) to produce water (H_2O):

$$2\left(H_2 \rightarrow 2e^- + 2H^+\right) \quad \text{(HOR)}$$

$$4e^- + 4H^+ + O_2 \rightarrow 2H_2O \quad \text{(ORR)}$$

$$2H_2 + O_2 \rightarrow 2H_2O \quad \text{(Net)}$$

Its PEM (electrolyte) controls the reaction by selectively passing protons while acting as a barrier layer to hydrogen, oxygen, and electrons (e^-), as shown in Figure 1.1. This forces the reaction to occur in two sub-reactions: the hydrogen oxidation reaction (HOR) whereby hydrogen is consumed and electrons and protons (H^+) are produced and the oxygen reduction reaction (ORR) whereby oxygen, electrons, and protons are consumed and water is produced. In order to complete the full reaction, the electrons must travel an external path. The path is provided by an external load which can harness the energy of the net reaction.

However, the cell has internal losses that cause heat generation and limit to the rate at which the electrons can do a given amount of external work. Some of the energy goes into making the reactions occur fast enough (activation losses), friction between the charge carriers (e^- and H^+) and the conducting materials (Ohmic losses), and transporting the reactants and products to the catalyst layer (concentration losses).

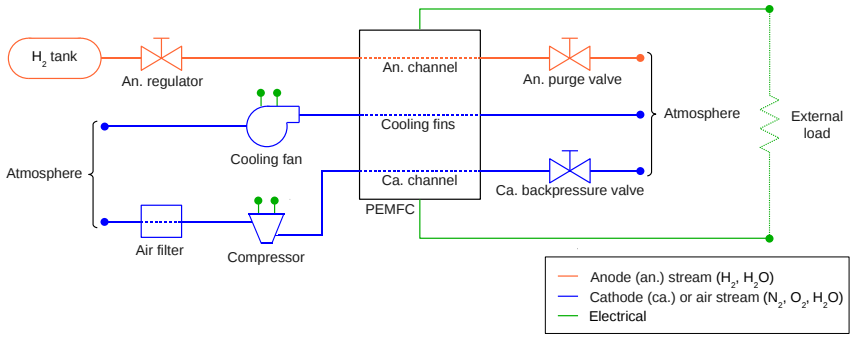
In order to operate, a PEMFC must be supported by other components, which are collectively called the balance of plant (BOP). The PEMFC stack and BOP are the basis of a complete PEMFC system like the one shown in Figure 1.3. Figure 1.4 shows the configuration of two PEMFC systems—one relatively simple and the other relatively complex. Even more complex PEMFC systems may include heat recovery [**?**] and fuel reformation.

Although PEMFC systems are promising, their cost and durability, and to a lesser extent, size and weight, must be improved to meet the desired standards for commercialization [**?**, p. 11]. The U.S. Department of Energy has outlined the numerous avenues that are being pursued to improve the PEMFC, BOP components, and PEMFC system as a whole [**?**]. The physical mechanisms of PEMFC degradation and failure are being determined and characterized through

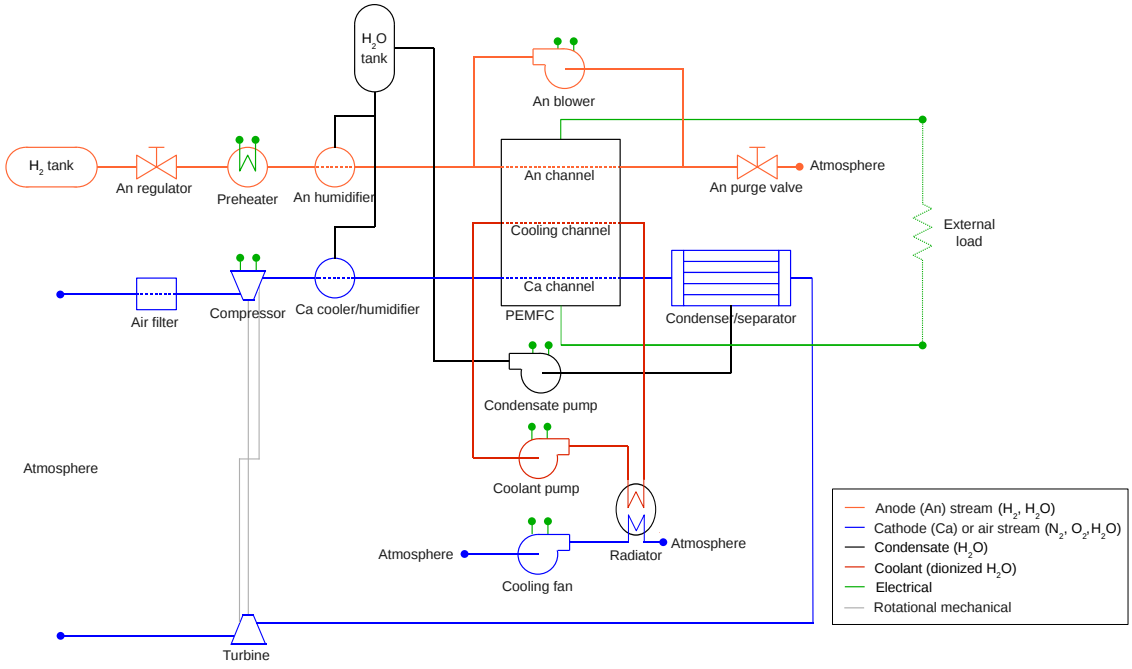
Figure 1.3: 100 kW PEMFC system used to power a bus. From Georgetown University, "Generation III Project," `http://fuelcellbus.georgetown.edu`, accessed Nov. 2011.

experimental and model-based investigations [**?**, pp. 3, 9, 32, & 40]. Novel materials and structures are being identified and developed for the core components of a PEMFC (Figure 1.1) as well as the seals between and around them [**?**, pp. 4–7]. These efforts seek to lower the cost of materials, improve thermodynamic efficiency (by increasing activity and conductivity), and improve robustness (specifically to air and fuel impurities, temperature and humidity variations, corrosive conditions, and power cycling). Design techniques and manufacturing processes are being developed to support the low-cost and high-throughput production of PEMs, electrodes, and flow plates [**?**, pp. 2, 5–6, & 29–30]. One goal is to more effectively integrate the PEM and electrodes (as a membrane electrode assembly) in order to minimize interfacial resistances, while at the same time allowing the raw materials to be reused or recycled [**?**, pp. 3–10].

The BOP components are being improved as well. New materials and concepts are being applied to heat exchangers, humidifiers, compressors, and turbines with the goal of reducing their weight, size, and cost [**?**, pp. 7, 10, & 32]. Since the air compressor places a significant internal electrical load on the PEMFC system, it is important to maximize its efficiency, and in some cases, a turbine is beneficial [61, p. 102]. Air filtration technology is being evaluated to allow PEMFCs to be used in off-road applications. Sensors, especially those for chemical composition, are being further developed for reduced cost and size and improved accuracy, reliability, durability, and dynamic response. [**?**, pp. 7]. The design of reformers and the operation



(a)



(b)

Figure 1.4: Configurations of two hydrogen-fueled (non-reforming), pressurized PEMFC systems where (a) the stack is air-cooled and (b) the stack is water-cooled, the anode is preheated and recirculated, the anode and cathode are both humidified, and the cathode exhaust is expanded through a turbine.

of PEMFC on reformate is also being improved [**?**, pp. 8–9], but in applications fueled by hydrocarbons rather than hydrogen, PEMFCs are less likely to be prevalent over high-temperature FC technologies that can accept those fuels directly (and perform internal reformation).

The final area of work considers how to improve the PEMFC system as a whole. Alternative PEMFC system configurations and design parameters are being considered that may allow the functions of the PEMFC system to be performed by fewer or simpler components, or that may entirely eliminate the need for certain functions [**?**, p. 10]. For example, one of the eight (or possibly more) possible methods for external humidification may be chosen, or the PEMFC can be operated within certain ranges of temperature and air flow rate where external humidification is not necessary [61, pp. 83–90]. Such choices must be guided by sufficiently accurate information, so PEMFCs are being tested to evaluate to their performance, durability, and other properties under various operating conditions, including hydrogen impurity [**?**, p. 9].

Mathematical models are used to assist many of these efforts to develop PEMFCs, but due to the complexity of the structures and the physical processes that occur within PEMFCs, specialized models are typically required for different situations. Many academic articles have been published with PEMFC models that are appropriate and useful for particular cell designs, operating conditions, and levels of fidelity (i.e., spatial, dynamic, or behavioral detail [**?**]) [**?**].[i] Ideally, variants of a common PEMFC model could be used for a wide range of research and development work, including physical investigation, model-based systems design, and model-based control. Such a model library could offer an open framework for PEMFC researchers to contribute their expertise and benefit from the collective knowledge of others.

Benefits of FC modeling [?**] **Issues in FCs: [**?**] **Move description of OO features from Chapter 4, discuss all the features from [**?**]

A broadly applicable PEMFC model library would need to contain models that are *physically representative*, meaning their predictions of behavior match reality (i.e., *accurate*) and their structure corresponds to the physical domain. Specifically and at a minimum, the static voltage-current predictions should be accurate over the following ranges of operating conditions:

[i] The next chapter provides a brief literature review.

- 300–900 mV electrical potential difference (per cell)[ii]
- 20–80 °C temperatures of flow plates and inlet gases (all varied together)[iii]
- 1–3.5 atm absolute anode/cathode outlet pressures (varied together)[iv]
- 0–100 % relative humidity at anode inlet[v]
- 30–70 % relative humidity at cathode inlet[vi]
- 14–100 % mean inlet/outlet oxygen concentration in dry cathode gas[vii]

The PEMFC model library should approximate the dynamic voltage-current response of actual cells at nominal operating conditions and varying large signal electrical currents (e.g., [**?**]). It should capture the operational effects of design parameters including component sizes and material properties (for hardware analysis and design) and should be capable of linearization (for control analysis and design). It should be able to describe relevant phenomena including electrochemical reactions, chemical/electrochemical transport, heat transport, and heat generation. It should also have variable fidelity so that it can be used for layer-, cell-, stack-, system-, or application-level simulations. Finally, it should be modular, meaning it should be possible to interconnect its submodels in various ways to build larger models analogous to the physical hierarchy. Unfortunately no current PEMFC model library can provide these features, let alone over the required range of operating conditions.

[ii] Low cell potentials (high electrical currents) are avoided in order to reduce the chemical/electrochemical transport losses. High cell potentials are avoided because they accelerate the corrosion that occurs due to electrical cycling [**?**, pp. 6–7].

[iii] The lower bound corresponds to start-up from room temperature. Nafion, the most common membrane material, dehydrates above ∼80 °C, which increases its protonic resistance [**?**].

[iv] Some PEMFCs operate at atmospheric conditions. PEMFC system efficiency is unlikely to increase above a pressure ratio of ∼3.1 [61, p. 107]

[v] For simplicity, some PEMFC systems do not have humidifiers (0 %). Other systems humidify the anode as much as possible without causing flooding to occur (up to 100 %).

[vi] The lower bound (30 %) corresponds to the relatively extreme case of operating the PEMFC without humidification in the Sahara desert on an average day [61, p. 78]. The cathode is generally not operated at saturated conditions; flooding would occur since H_2O is also produced in the cathode.

[vii] The lower bound corresponds to a stoichiometric ratio (stoich.) of 1.5. The risk of starvation increases as the ratio approaches 1.0. PEMFCs are also operated on pure oxygen in applications such as unmanned underwater vehicles (UUVs).

1.2 Overview of the Research

1.2.1 Research Questions and Objectives

The research seeks to make steps towards achieving the ideal PEMFC model library described above. The following questions will be addressed:

1. How can we model all the relevant physical phenomena of fuel cells to support the analysis and design of PEMFC systems, inclusive of hardware and controls?
2. How can the equations be structured so that they can be symbolically manipulated to improve computational speed and to allow linearization for control design?
3. Which combinations of accuracy and speed can be achieved by adjusting fidelity?

The high-level objectives of the research are (i) to establish physically representative equations for modeling PEMFC behavior, (ii) to evaluate the equations' static and dynamic accuracy, and (iii) to evaluate the effect of modeling assumptions and lengths of spatial discretization on accuracy and speed of computation.

1.2.2 Modeling Approach

The model is temporally continuous and spatially discrete. Transients are modeled in terms of differential algebraic equations (DAEs), or implicit ordinary differential equations (ODEs) combined with algebraic constraints. The integrator is built into the simulation tool, which allows the source code to focus on the physical phenomena rather than the solution. It also improves the robustness of the simulation, since advanced integration algorithms are available [**?**].

Spatial variances are modeled in terms of differences rather than derivatives as in partial differential equations (PDEs). As stated by Mattiussi [**?**], this representation has three advantages: (i) it provides a unified perspective that is appropriate for many theories, (ii) it directly correlates the discretization of the physical region and the structural properties of the applied theories, and (iii) it is based on intuitive geometrical and physical concepts that help distinguish the numerical methods (e.g., FDM, FVM, FEM, etc.) and the underlying theories.

The model equations are expressed in a *declarative* language that preserves the simultaneous mathematical nature of the equations. By definition, an equation declares a relation

between two expressions without implying mathematical causality (i.e., assigning independent and dependent variables). The solver, which is built into the simulation tool, automatically translates the equations into sequential mathematical assignments which do imply causality. Traditional models are developed directly in this *imperative* representation. The assignment operations are organized to form algorithms within functions or blocks with predetermined input/output assignments.

Declarative = acausal = physical-interaction [?**] **Imperative = causal = signal-flow [**?**]

The use of declarative language has three main advantages for modeling physical systems. First and foremost, it best represents the nature of physical behavior and preserves the meaning of physical laws [**?**, **?**, **?**, **?**]. Although current leads voltage in a electrical capacitor, the current does not cause the voltage to change any more than the change in voltage causes a current. Placing the causality assignment in the capacitor's physical description is to suffer from the "post hoc ergo propter hoc (it happened before, hence it caused) fallacy" [**?**]. This observation extends to fuel cells [**?**]. Declarative language allows the relationship to be expressed directly, without causality.

succinctly: "Physical conservation laws do not apply in these applications because the same information can flow (be copied) to multiple components, while physical things cannot." [**?**]

The second advantage is that declarative models are more intuitive than imperative ones. This is demonstrated by Figure 1.5, which shows imperative and declarative models of the same electrical circuit. The connections of the imperative model (Figure 1.5a) represent signals. The type of signal (in this case voltage or electrical current) depends on the connection's context within the circuit, since the block for each electrical component receives voltage and transmits electrical current or vice versa. Kirchhoff's voltage and current laws (KVL and KCL) are explicitly represented as difference and summation blocks, and this distracts attention from the blocks which represent the constitutive equations of the capacitor, inductor, and resistors. In contrast, the connections of the declarative model (Figure 1.5b) represent wires which imply the topological equations (KVL and KCL). The diagram shows how the components would be actually assembled.

easier to make mistakes with imperative models [?**]

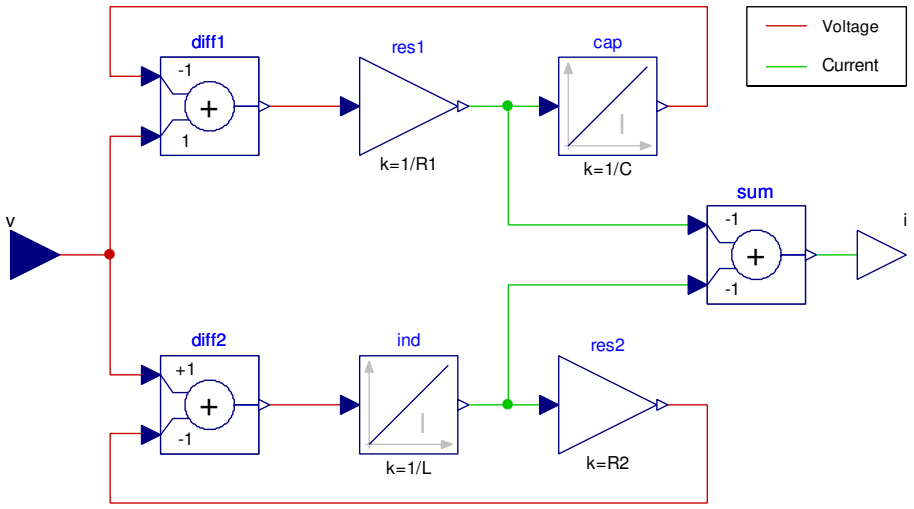
The third advantage is that declarative models are flexible because they preserve the information necessary to perform symbolic manipulation. Powerful modeling tools (e.g., Dymola [**?**]) exist that can solve a model for the imposed causality, linearize a model, partition a dynamic model into the most numerically efficient systems of algebraic equations (i.e., resolve algebraic loops through tearing), and perform index reduction (i.e., eliminate structural singularities) [**?**, **?**, **?**]. In addition, methods are being developed for analytical model order reduction (MOR) [**?**]. Returning to the electrical example, the declarative model of Figure 1.5b independently maintains information about the circuit (capacitor, inductor, resistors, and their connections) and the causality imposed on it by the boundary condition (voltage source). If the boundary condition is changed (e.g., current source instead of voltage source), a simulation solver can automatically change the causality as needed. However, the imperative model of Figure 1.5a must be manually re-solved and reconfigured as shown in Figure 1.6. The correlation is not obvious and this makes model development and usage difficult. It is not practical, especially for complex systems, to maintain multiple versions of a model for the sake of causality. Automatic linearization is helpful in evaluating dynamic characteristics and in control techniques such as model predictive control (MPC). Algebraic loops tend to occur in the representations of complex physical systems; therefore, it is helpful that declarative modeling tools are able to handle them in a robust manner. Index reduction is important in applying assumptions to the proposed PEMFC model, as will be discussed in Chapter 4.

imperative models less reusable [?**]

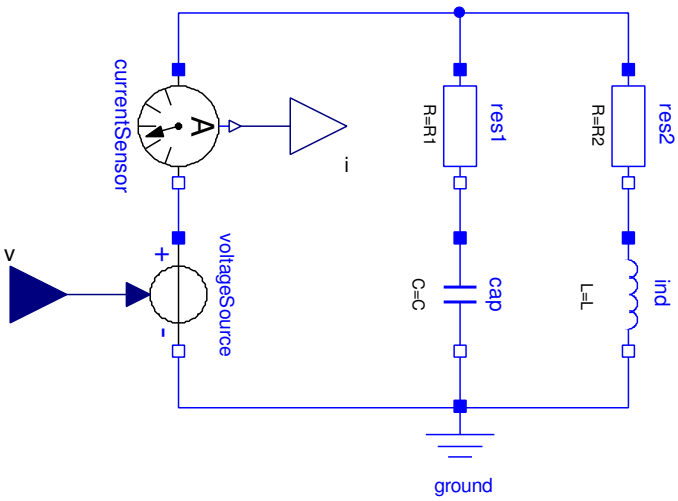
The major disadvantage of declarative models is that they are not well-developed for domains, e.g., chemistry. Also, imperative simulation tools are much more prevalent [?**].

1.2.3 Scope

The fuel cell model presented in this dissertation is rather low-level. It is generally based on first principles (e.g., momentum balances). An initial goal was to evaluate a fuel cell model at the fuel cell system level. However, it was determined that it was first necessary to develop alternative methods of modeling multi-species fluids and properly represent fundamental processes such as mixed advection and diffusion within a declarative framework. Electrochemical



(a) Imperative.



(b) Declarative.

Figure 1.5: Imperative and declarative and imperative representations of an electrical circuit [**?**].

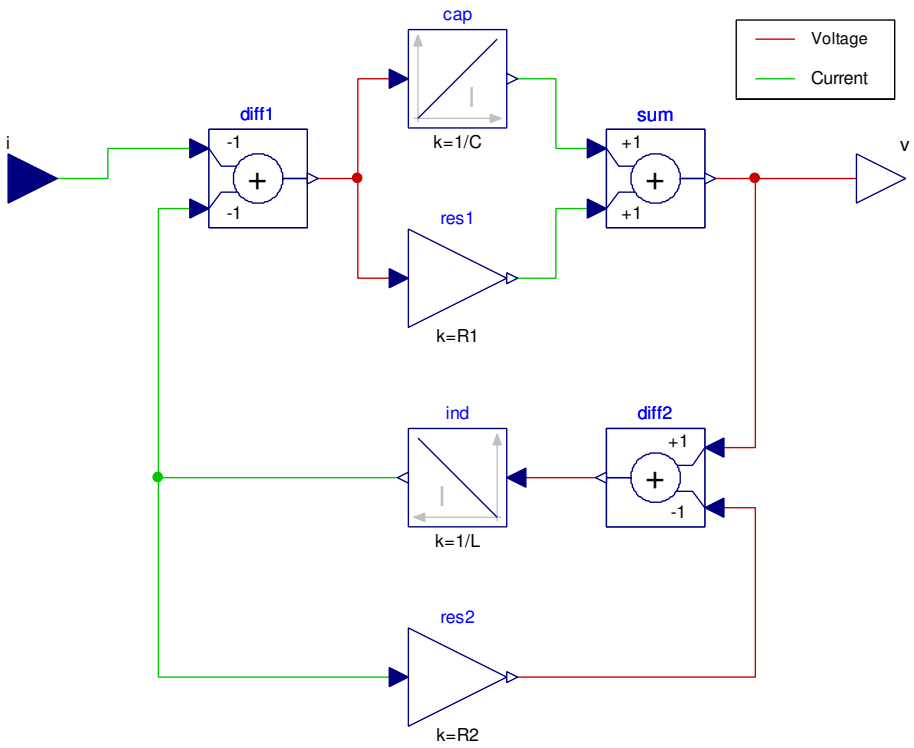


Figure 1.6: Inverse imperative representation of the circuit in Figure 1.5.

devices and processes have not yet been described in a manner that at once (i) is implementable within declarative language, (ii) can be factored to have physically representative model partitions, (iii) include all of the relevant phenomena in a fuel cell, (iv) is dynamic, and (v) is true to the underlying physics(see [**?**,**?**]). The research questions and objectives have been established in this context.

Yet it is known that declarative modeling is well-suited for system design [**?**,**?**,**?**]. The fuel cell model has been developed with this in mind. The model library is highly modular and reconfigurable in terms of spatial resolution and dimensionality, choices of chemical/electrochemical species, and assumptions regarding property correlations and physical phenomena. The tradeoffs between accuracy, fidelity, and computational speed are evaluated in Chapter 7. This provides an estimate of the scalability of the model for fuel cell system analysis.

CHAPTER 2

BACKGROUND

CHAPTER 3

FUNDAMENTALS OF THE MODEL

CHAPTER 4

IMPLEMENTATION OF THE MODEL

CHAPTER 5

STATIC ANALYSIS

CHAPTER 6

DYNAMIC ANALYSIS

CHAPTER 7

COMPUTATIONAL PERFORMANCE

CHAPTER 8

CONCLUSIONS

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