

# Computational Fuel Cell Dynamics

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Abstracts

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## **Capillary-Driven Flow in Liquid Filaments Connecting Orthogonal Channels**

Capillary phenomena plays an important role in the management of product water in PEM fuel cells because of the length scales associated with the porous layers and the gas flow channels. The distribution of liquid water within the network of gas flow channels can be dramatically altered by capillary flow. We experimentally demonstrate the rapid movement of significant volumes of liquid via capillarity through thin liquid films which connect orthogonal channels. The microfluidic experiments discussed provide a good benchmark against which the proper modeling of capillarity by computational models may be tested. The effect of surface wettability, as expressed through the contact angle, on capillary flow will also be discussed.

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## **Impedance as a diagnostic tool for studying fuel cells**

We will start by showing some CFD simulations of current distribution on a fuel cell. The current distribution behaves differently under different operating conditions and we will try to explain this behavior. This will lead us to consider impedance spectroscopy as a tool to investigate some of the critical effects that impact current distribution. A short explanation of impedance methods will be given along with a discussion of how to interpret impedance data in the context of current distribution.

Special emphasis will be given to the high frequency resistance (HFR) as a tool for understanding membrane humidification. Other impedance applications include assessing proton resistance in the porous cathode, kinetic resistance of the cathode electrode, and the relative contribution of gas transport resistance to voltage losses.

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### **The Autohumidification Polymer Electrolyte Membrane Fuel Cell**

A PEM fuel cell was specially constructed to determine kinetics under conditions of well-defined gas phase composition and cell temperature. Steady state multiplicity was discovered in the autohumidification PEM fuel cell, resulting from a balance between water production and water removal. Ignition was observed in the PEM fuel cell for a critical water activity of 0.1. Ignition is a consequence of the exponential increase of proton conductivity with water activity, which creates an autocatalytic feedback between the water production and the proton conduction. The steady state current in the ignited state decreases with increasing temperature between 50 – 105°C. At temperatures of > 70°C five steady states were observed in the PEM fuel cell. The steady state performance has been followed with variable load resistance and hysteresis loops have been mapped. The dynamics of transitions between steady states are slow 10<sup>3</sup> - 10<sup>4</sup> s. These slow dynamics are suggested to result from a coupling of mechanical and chemical properties of the membrane electrode assembly due to swelling of the membrane with water absorption.

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### **1+1 Dimensional Model of Technical PEFC Single Cell with Focus on Water Transport**

The performance of polymer electrolyte fuel cells strongly depends on the cell water management. Based on a literature approach for the cell water distribution, a full cell model realized in a 1 + 1 dimensional approach was developed. The model can describe the co- and counter-flow regimes in a cell. A combination of these regimes was used, to describe the water management and local current densities of the given

technical cell flow field. The calculations allowed identifying the contributions of the different loss mechanisms with respect to operating conditions. The model was verified with local current measurement data from the described cell.

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### **Membrane Swelling and Proton Transport in Nafion**

The development of an inexpensive proton-exchange membrane (PEM) that has a high proton conductivity at low relative humidity (RH) and high temperatures, a low fuel/oxygen permeability, and a high chemical, thermal and mechanical stability is a dream of many a polymer scientist and will substantially impact the large scale deployment of PEM fuel cells. The design of such a PEM would be aided by a quantitative understanding of the sorption and transport characteristics of Nafion, the current workhorse and a well-characterized membrane. A physically plausible model is, thus, developed that provides a basic framework for the design of a proton-exchange membrane with desirable characteristics.

A thermodynamic model is developed<sup>1</sup> for Nafion swelling that accurately describes the membrane sorption at various RH and also provides a logical explanation for the so-called Schroeder's Paradox, namely the difference in swelling in saturated vapor versus liquid. The sorption model is based on the premise that the swelling is controlled by the adsorbate chemical potential which in turn is affected by the osmotic pressure determined by the polymer matrix elasticity as well as the chemical interaction between the adsorbate and the polymer. This thermodynamic sorption model is coupled to a phenomenological transport model<sup>2</sup> based on the dusty-fluid model for predicting the Nafion<sup>®</sup> conductivity as a function of RH and temperature.

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## **Analysis of Some Aspects of Water Transport in a PEMFC Using 3D Multiphase Simulations**

A description of the two-phase PEMFC model implemented at UVic using a CFD code will first be provided, with a discussion of the various modeling assumptions. An analysis of water transport will be presented based on simulations of a 3D section of a cell, including both anode and cathode, operating with fully humidified inlet reactant streams. We will focus on results that help understand the underlying mechanisms of phase change due to the coupling of temperature, saturation pressure, phase change, pressure drop inside the GDE, and reactant partial pressure. Some of the open issues to be considered in further developments will also be discussed, including the “proper” determination of transport parameters and the resolution of the high current density regime.

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### **A detailed numerical Model for DMFC: Discretization and Solution methods**

The analytical description of the WIAS DMFC model is based upon systems of partial differential equations which describe physical phenomena as catalytical reactions, chemical reactions, diffusion, multiphase flow, convective transport. The model has been implemented in a research code developed by the Weierstrass Institute. The code allows for both transient and stationary simulations, parameter variations and measurement fits on one-, two- and (with some restrictions) three-dimensional unstructured meshes.

More precisely, we will focus on

- + The Voronoi box based finite volume (control volume) method for space discretization for nonlinear convection-diffusion problems
- + Stability and existence analysis of the discrete problem in the scalar case
- + Generalization of the discretization ansatz to systems of convection-diffusion-reaction problems (analysis is still unsolved)
- + Solution methods for the nonlinear and discretized problems
- + API and software framework
- + Outlook

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## **A detailed numerical model describing DMFC: species transport, reaction kinetics and temperature feedback**

The Species transport in our DMFC model is described by

- + Stefan-Maxwell Diffusion of a gas mixture in a porous medium,
- + Two-Phase (water/gas) flow in a porous medium,
- + Transport of dissolved species in water,
- + Transport of charged species.

In the model gases and fluids interact via the total gas pressure (the related saturation and relative permeabilities), and evaporation/condensation. The two phase flow is influenced by mixed wettability effects due to the Teflon admixture. This is reflected in a new parametrization of the pressure saturation curves and in the boundary conditions.

The reaction kinetics influences the function of DMFC's seriously. Three different kinetic models are used to describe the electrochemistry and the competition for the finite number of catalytic sites: reactions of CH<sub>3</sub>OH in presence of Pt/Ru or a Pt catalyst and O<sub>2</sub> in connection with Pt. The adsorption models result in equations having neither a unique stationary solution for the single reaction nor for the complete cell. Assuming "ideal transport" and two reactions only (with one non monotone reaction rate in dependence of the electrochemical potential) results in an easily to classify, but nonunique, situation in the stationary case. A reaction model describing the cathodic reactions of H<sup>+</sup>, O<sub>2</sub>, CH<sub>3</sub>OH for a large range of concentrations, potentials, and temperatures is still an open question.

Accordingly to the goal to include many of the feed-back effects the reaction models depend on temperature. The energy balance has been introduced accordingly: the different spatially separated reaction steps are taken as individual sources into account.

The model assumes fast reactions (stationarity) at present. The numerical algorithms are based on an inner Newton's method combined with imbedding (which yields the occupation numbers of the catalytic sites) and an outer one based on the analytic Jacobian of the discrete equations for the outer variables (mobile species). The outer Newton process is used together with a direct method and an imbedding scheme to solve the stationary or time dependent equations describing the DMFC. The spatial discretization is based on upwinded finite volume schemes for simplices forming a Delaunay grid.

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### **Electrochemical Potentials in Steady-State Fuel Cell Modelling**

Component electrochemical potentials can be used to describe steady-state diffusion-reaction-conduction processes in electrochemical systems. This presentation will discuss the use of these potentials in modelling MCFC (molten carbonate fuel cell) cathodes and PEM cells. Topics discussed will include how the component potentials relate to concentrations, currents, etc., and some of the results that can be obtained using these potentials.

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### **Conduction of water and protons through carbon nanotubes**

Recent experiments and molecular dynamics simulations show that water can fill the interior channels of carbon nanotubes despite their low polarity. Based on detailed molecular dynamics simulations on classical and quantum energy surfaces, I will analyze the factors that determine the thermodynamics [1] and kinetics [2] of water filling narrow nonpolar channels; the mechanism and rate of water transport through such channels [1,3,4]; and the mechanism and rate of proton transport along water chains confined into carbon nanotubes [5].

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### **Advance PEM Fuel Cell Models and Application to PEM Commercial-**

## ization Challenges

My talk will focus on some unique applications with selecting unit cell modeling parameters and applying them towards global marketing targets such as improved system efficiencies, fuel economy, reducing component and system costs, and impact on clean emissions. Innovative PEM fuel cell models being developed today focuses on discrete applications for modeling electrochemical behavior and characterizing mass transport mechanisms in cell structures. Examples such as membrane modeling, catalyst, mass transport, thermal models dive into specifying key unit cell parameters for improving performance. I will discuss a few ways we might use these same models to extrapolating interesting comparisons and benefits that PEM fuel cells offer for the power market.

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## Flow and Reaction in Solid Oxide Fuel Cells

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## Modeling Carbon Monoxide Poisoning And Oxygen (Air) Bleeding in PEM Fuel Cells

Polymer electrolyte membrane (PEM) fuel cell has increasingly become the potential choice of zero-emission power source for transportation applications, in place of the internal combustion engine. However, the use of pure hydrogen as the fuel in transport applications has several challenges, such as onboard storage and a lack of hydrogen distribution infrastructure. Therefore, in the near term, the hydrogen for a PEM fuel cell in transportation applications would have to be generated on board by reforming a liquid hydrocarbon, such as methanol. Unfortunately, the reformation of a hydrocarbon fuel produces carbon monoxide, which at the low operating temperature of a PEM fuel cell severely poisons the electrochemical reactions; the energy conversion efficiency and output power are reduced significantly such that the PEM fuel cell may no longer be viable as the zero-emission alternative to the existing technology. Therefore, the issue of carbon monoxide poisoning is a significant hurdle to the commercialization of PEM fuel cells for transportation applications. In the

present study, a mathematical model has been formulated for the performance and operation of a PEM single cell. This model incorporates all the essential fundamental physical and electrochemical processes occurring in the membrane electrolyte, cathode catalyst layer, anode catalyst layer, electrode backing and flow channels. A special feature of the model is that it incorporates the processes of adsorption, desorption and electrooxidation of both carbon monoxide and hydrogen at the anode catalyst layer and as a result, the model can simulate a carbon monoxide poisoned PEM fuel cell. In addition, the heterogeneous catalysis of hydrogen and carbon monoxide with oxygen is included for the simulation of oxygen or air bleeding. The model predictions have been compared with the existing experimental results available in the literature for various cell operating temperatures, pressures and carbon monoxide concentrations; and excellent agreement has been demonstrated between the model results and the measured data for the cell polarization curves. Hence, this model can be used to illustrate the effect of carbon monoxide on PEM fuel cell performance. Simulations with oxygen and air bleeding indicate that a threshold amount of oxygen or air bleeding exists; any increase in the amount of bleeding above the threshold amount results in no further mitigation of CO poisoning. The threshold amount of oxygen or air bleeding is a function of cell current density, with a greater cell current density demanding a larger threshold amount of oxygen or air bleeding.

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### **Energetic Variational Method in the Study of Multiple Component Fluids**

In this talk, I will review the theory of diffusive phase field method to study the free interface in multiple component fluids. We will employ an energetic variational method to derive the coupling hydrodynamical system. The focus will be to study the interaction between the flow transport and the induced elastic stress (surface tension in the isotropic cases). The method can be generalized to the cases of more complicated interfacial effects, such as the Marangoni effect due to the temperature of the concentration of surfactant particles. Several analytical as well as numerical results will be presented.

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## Rivulets

Abstract

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### **Ionic Diffusion Through Microscopic Regions: From Molecular Description to Continuum Equations**

The diffusive motion of particles through a microscopic region, as in ionic permeation through protein channels of biological membranes, or through the nanopores of polymer electrolyte membranes of fuel cells, is an important phenomenon in many diverse fields. In the case of protein channels, permeation occurs on a time scale of micro- to milli-seconds, far longer than the femto-second time scale of atomic motion. Since direct molecular dynamics simulations are not possible for such long time scales, a description on a coarser scale is unavoidable. Standard continuum formulations based on macroscopic conservation laws, such as the Poisson-Nernst-Planck equations, cannot be assumed valid in narrow channels, where diffusing ions interact with each other. This leads to the more general coarse graining problem: The description of the diffusive motion of interacting particles in a confined region connected to a bath by averaged continuum equations. In this talk we present a mathematical averaging procedure that, starting from a Langevin model of ionic motion, yields effective continuum equations and boundary conditions. Our main result is a coupled system of Poisson and Nernst-Planck type equations, containing conditional and unconditional charge densities, coupled to conditional potentials. The proposed system of equations differs from the standard PNP system in two important aspects. First, the force term in the Nernst-Planck equation depends on conditional densities, which are the non-equilibrium analogues of the well studied pair correlation functions of equilibrium statistical mechanics. Thus our equations express the finite size of ions, which are known from equilibrium theories to cause first order effects on bulk properties of electrolytes. Second, the force in the Nernst-Planck equation contains an additional term, the dielectric self force on a discrete ion, due to the surface charges induced by that ion at dielectric interfaces. This non-negligible force term was neglected in continuum theories. Finally, we note that our work can also serve as a part of a multi-scale analysis, in which the local diffusion coefficients and pair correlation functions of our effective equations are the output of molecular dynamics simulations.

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### **Improving HFC performance through optimization of channel/GDL transmission coefficient**

Assuming that the porosity of GDL is fixed, the channel-GDL transmission coefficient  $S$ , is the only quantity coupling the speed in channel and GDL. We will discuss how to define this coefficient, thus relaxing it as a 2D function in channel-GDL interface, in order to get better HFC performance. We will present a method that to any given coefficient  $S$  associates a porous domain (GDL) structure. We will present different numerical results that show the porous domain structure corresponding to a given coefficient  $S$ .

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### **Diagnostics of Liquid Water Flooding in PEMFC Electrodes**

## Understanding Proton Conduction in the Polymer Electrolyte Membrane through Molecular and Statistical Mechanics Modeling

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For the PEM fuel cell to be successfully integrated into the mass-market new materials will need to be developed, including: electrocatalysts for the fuel and air electrodes and the proton conducting membrane [1]. New materials possessing improved properties will emerge as a result of a collaborative effort between experimentalists, engineers, and theorists, the later doing both device and materials modeling. For the physical and chemical modeling of materials to play a role in the suggestion of new materials the modeling must be at the nano- and even molecular scale and ideally it should not be phenomenological but rather from “first principles”.

The hydrated PEM is an inhomogeneous material the morphology of which is not well characterized. As such it is a system that must be examined through modeling at several distinct length and time scales. Our approach has been to theoretically examine proton conduction in the PEM at three distinct length and time scales implementing three different approaches [2-9]. The hierarchy of this multi-scale modeling is as follows: (1) proton dissociation and hydration of hydrophilic groups in the membrane using *ab initio* molecular orbital theory; (2) local proton dynamics ‘near’ (between) the fixed sites studied with *ab initio* (quantum) molecular dynamics; and (3) proton diffusion and the state (permittivity) of the water within a single membrane pore or channel applying both equilibrium and non-equilibrium statistical mechanics.

This talk will present new results and analysis of proton conduction derived from the three approaches described above and at various degrees of hydration with various membranes.

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### **The development of Variational Methods for the investigation of Ion Transport in Hydrated Polymer Electrolyte Pores**

Nanopores that constitute the main conduits of transport in polymer electrolytes present some unique challenges to the theoretical physicist. Although the numbers of molecules are few, compared to the bulk phase, the small volume available forces these molecules to reside in very close proximity to each other. As a consequence many of the standard analytical techniques based on perturbation and graph theoretical methods are no longer helpful. In the final analysis one is forced to either depend on numerical or variational techniques. In this seminar a variational method that has potential applications in solving integral equations, particularly the Ornstein-Zernicke equation, will be presented.

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### **An overview of PEM fuel cells:Mathematical issues**

This introductory talk will outline the basic functionality of pem fuel cells, from multiphase flow in the hydrophobic gas diffusion layers to ion conduction and electro chemistry in the membrane and catalyst layers. The major issues of device modeling will be addressed. We will point out areas which are ripe for mathematical investigation: morphology of polymer membranes underhydration, capillary effects in the catalyst layer and GDL-channel interfaces, ion channel modeling in the membrane, and the need for adaptive codes to handle stiffness, high aspect ratios, and moving interfaces.

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### **Ion Exchange Funnelling in Modified Heterogeneous Ion Exchange Membranes**

Inexpensive highly permselective heterogeneous ion-exchange membranes usually suffer from high polarizability by a dc current. According to recent experiments, this deficiency may be considerably reduced by casting on their surface a thin layer of crosslinked polyelectrolyte, slightly charged with the same sign as the membrane's charge. Our talk is concerned with this effect. Concentration polarization of a permselective heterogeneous ion-exchange membrane by a dc current is determined by geometric factors, such as, the typical size of the ion-permeable "gates" at the membrane surface relative to the separation distance between them and the diffusion layer thickness. The main quantitative characteristic of polarizability of a heterogeneous membrane is its voltage/current curve with its typical saturation at the limiting current, which is lower than that for a homogeneous membrane. We present a two-dimensional model of ionic transport in a diffusion layer at a heterogeneous ion-exchange membrane modified by a homogeneous ion-exchange layer cast on the membrane surface. A numerical solution of the respective boundary value problem shows that, indeed, adding even a very thin and slightly charged layer of this kind increases the value of the limiting current, to that of a homogeneous membrane. What differs, for different values of coating parameters, is the form of the voltage/current curves but not the value of the limiting current, namely: the thinner is the coating and the lower the fixed charge density in it, the "slower" is the approach of the limiting current. In order to explain this feature, a simple limiting model of modified membrane is derived from the original two-layer model. In this limiting model, asymptotically valid for a thin coating, solution of the ionic transport equations in it is replaced, via a suitable averaging procedure, by a single nonlinear boundary condition for the membrane/solution interface. Rigorous analysis shows that the aforementioned property of the limiting current is an exact mathematical feature of this limiting model, when the underlying physical phenomenon is the funneling of counterions by the charged layer from the impermeable parts of the membrane towards the "entrance gates".

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### **Modeling hydrophobicity in a porous fuel cell electrode**

Water management is a fundamental issue in the the performance of proton exchange membrane fuel cells. Hydrophobic materials are an essential component of most water management strategies, and ensure that the liquid water produced by the driving reaction does not remain to block reaction sites. I will describe some aspects of modeling the flow of liquids in hydrophobic porous media, which has appeared

in the soil transport literature. I then develop a model for a hydrophobic fuel cell electrode which couples gas and liquid transport along with condensation. Numerical results are presented that demonstrate the applicability of the model to fuel cell systems.

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### **A Simple but Comprehensive PEM Unit Cell Model**

We present a minimal model for PEM unit cells with straight channels in steady state conditions capable of predicting: current density profiles, local and total water crossover, effects of inlet humidity, and voltage sensitivities. The model is capable of describing co-flow and counter-flow operation. In the model, channel flows are represented by average molar fluxes. The membrane is represented in some detail, with proton concentration determined by a local chemical equilibrium, and nonlinear water and proton diffusivities. Cathode electrochemical losses are considered based on standard Tafel relationships. The model contains only three main fit parameters: exchange current density, a parameter representing oxygen transport losses from the channels to the catalyst sites, and a parameter representing limitations on water transport from the catalyst to the channels. Techniques for effectively fitting these parameters to experimental data are outlined. Extensive comparison to data from the Ballard Mk9 hardware has been conducted.

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### **Multilevel adaptive methods for partial differential equations**

This talk will be devoted to explaining some basic ideas on multilevel iterative and multilevel grid adaptation methods for solving partial differential equations and to presenting a few recent results, including a new sharp convergence theory on the general subspace correction iterative methods, a new a posteriori error estimator and some applications.

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### **PEMFC Device Modeling: Using CFD Models to Understand PEM Fuel Cell Behavior**

The design, operation, and control of PEMFCs depend on proper water management, the rates of poisoning and recovery during carbon monoxide transients, and the response of the system to transient load changes. Three-dimensional steady-state and transient models for serpentine flow fields (SFFs) based on computational fluid dynamics (CFD) software and user supplied subroutines are being used in our laboratory to understand these issues. These models and their constitutive equations are verified with current-voltage and water balance data from laboratory-scale cells. Predictions will be discussed for the effects of flow field design, gas diffusion layer permeability, inlet humidity conditions, and heat transfer on the distributions of current and water in a PEMFC. The results of transient simulations of rapid voltage changes will be used to explain current overshoot and undershoot data.