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[KINETIC ISOTOPE EFFECT STUDIES OF PARA - SUBSTITUTED-N,N- DIMETHYLANILINES]

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VIRGINIA TECH

Abstract. According to the published literature (Dinnocenzo, Karki, & Jones, 1993), N-benzyl-N-cyclopropylamines may be oxidized by Cytochrome P450 (CP450) via two proposed mechanisms: the hydrogen atom transfer (HAT) mechanism or the single electron transfer (SET) mechanism. During the SET mechanism, a catalytic intermediate is formed, the dimethylaniline radical cation. These dimethylaniline radical cations are believed to undergo a subsequent deprotonation step in the presence of a base. In chemical model studies with the acetate anion our preliminary electrochemical studies show that a SET mechanism is actually occurring. A mechanistic study performed by nanosecond Laser Flash Photolysis (LFP) to aid in elucidation in the mechanism of this reaction by determining the Kinetic Isotope Effects (KIE) for deuteromethyl compounds was performed. A KIE of 2.5 ± 1.6 was observed suggesting that this method is incapable of accurately assessing rate constants for reactions on the time scale observed for these compounds. In summation, LFP studies did not provide significant evidence for or against the mechanism of the acetate anion with dimethylaniline radical cation.

Exploring Chaos using Numerical Simulations of Simple Models

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Abstract

Many physical systems present complicated behavior that is difficult to predict because of nonlinear chaotic dynamics. These systems include the weather, the excitation of heart tissue, convective flows, chemical reactions, and tip oscillations in atomic force microscopy. Complex systems are important and poorly understood, but very little is understood about even the simplest models of chaotic dynamics. Our strategy was to develop programs to demonstrate the principles of chaos using simple models. The programs were designed to numerically solve, show the results of, and evaluate quantitative data for chaotic models. By programming applets in the JAVA language and posting the resulting applications on the internet, the demonstrations were made available to a wide range of users. The resulting website is found at www.me.vt.edu/chaos. It contains demonstrations of the von Koch curve and the Lorenz equations, as well as descriptions of spatially extended models. Each model presents important features associated with chaos with increasing complexity.

A Novel Polystyrene Derivative Designed for PEMFCs

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1. Introduction

PEM fuel cells present many attractive qualities that insure their future as a viable energy conversion technology. They constitute a more efficient and environmentally friendly alternative to the internal combustion engine, whose fuel has been a financial, political, and ecological concern for several decades. Fuel cell technology has been proven feasible in many respects [1], but the central component of a PEM fuel cell, the polymeric proton exchange membrane, must be optimized in order for the PEMFC to become fully integrated into the market. PEMs must exhibit satisfactory performance in many areas, showing high ionic conductivity, electrical insulation, thermal stability, mechanical strength, and chemical stability, as well as low cost and manageable swelling upon hydration [2].

To date, poly(perfluorosulfonic acid) polymers, namely DuPont's Nafion[®] (**Figure 1**), have been the benchmark according to which other proton-conductive materials are judged. As Nafion[®] becomes better understood, however, it is becoming clear that it will not be able to meet the Department of Energy's desired operating temperature of 120°C due to decreased performance

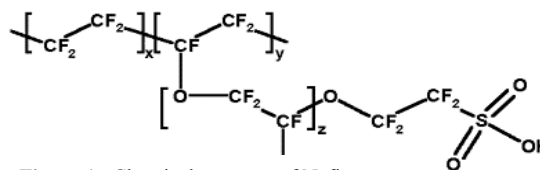


Figure 1: Chemical structure of Nafion

at higher temperatures, namely lower protonic conductivity due to membrane dehydration and lower mechanical strength [3]. This, coupled with its high price (~\$160 kW⁻¹, far from the desired \$10 kW⁻¹) and the difficulties inherent in working with fluorinated compounds, necessitates research in other types of ionomers [1]. The goal is to design new polymers with same conductivity as Nafion[®], but cheaper and capable of operation at higher temperatures [4].

Many types of polymers have been studied as alternatives to Nafion[®]. Most involve the presence of the sulfonic acid or carboxylic acid functionalities to form an ionic environment in which water can transport protons through the membrane [11]. The sulfonation process is quite versatile; a variety of sulfonating agents can be easily employed either before or after polymerization in many reaction conditions, and sulfonation can impart to a polymer many important properties, such as hydrophilicity [6]. Also, perfluorinated polymers provide extra resistance to degradation by radicals present in the fuel cell environment, as well as enhanced stability at higher temperatures and increased proton conductivity [7,8].

Some promising materials involve polystyrene derivatives, polymers with strictly aryl backbones (i.e. poly(ether ether ketone), or PEEK), and various other condensation polymers. Hickner et al [3] explores many of these options in a review of alternatives to Nafion[®]. Examples include acid-doped polybenzimidazole, polyphosphazene, poly(arylene ether sulfone), polyimide, polysulfone, among many others [1,3,7]. **Figure 2** shows the chemical structure of a

promising poly(arylene ether sulfone), BPSH-xx, where xx is the ratio of sulfonated to unsulfonated activated halide starting material.

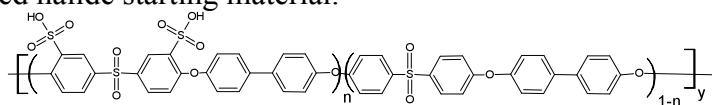


Figure 2: Chemical structure of BPSH-xx

PEMs containing styrene and its derivatives also occur commonly in the literature and likewise present a very diverse palette of chemical possibilities due to the ease of manipulation and polymerization of styrene [1-16]. Hickner et al [3] report a variety of polymerization techniques possible with styrene. These include grafts of PSS onto PS chains, and various block copolymers. Two of these have received substantial coverage in the literature [1,3,7]. Sulfonated styrene-ethylene-butylene-styrene (SEBS) from Dais Analytical Chen includes aliphatic blocks that increase the flexibility of the polymer, affording better attachment to the electrode and high proton conductivity, but at the expense of mechanical and chemical stability. Chen et al [1] researched composite membranes of SEBS and a crosslinked PSS ion exchange resin, finding decreased swelling due to hydration, more resilient mechanical and chemical stabilities, slower rates of degradation, and increased IEC (although ionic conductivity remained unchanged) compared to a normal PSS membrane. Another commercial polystyrene derivative is BAM3G, produced by Ballard Advanced Materials Corporation. This material is composed of

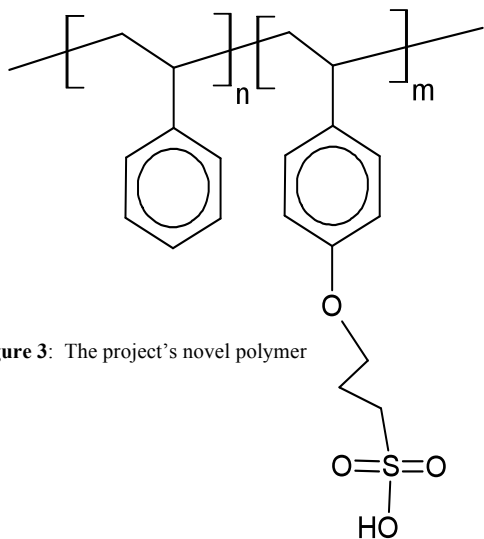


Figure 3: The project's novel polymer

α,β,β -trifluorostyrene monomer and has exhibited superior durability and better performance than Nafion[®] in some conditions [7]. Shin et al [9] reported on PSS/PTFE composites for use in DMFCs, and found that water uptake could be effectively controlled and that the methanol permeability of these polymers was lower than that of Nafion[®].

This project concerns attaching perfluorosulfonic acid sidechains (via trials with 1,3-propane sultone) to a derivative of polystyrene, which is obtained through copolymerization of styrene and 4-acetoxystyrene, followed by deacetylation to form poly(styrene-*co*-vinylphenol) (PS-*co*-PSOH) (**Figure 3**) [10-13,27]. The extra mobility afforded to the sulfonic functionalities is believed to allow for greater ionic aggregation, yielding better proton conductivity in fuel cell conditions.

Effects of solvent-casting conditions on the final properties of disulfonated poly(arylene ether sulfone) copolymer films for fuel cell proton exchange membranes

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Materials and Processes for Proton Exchange Membrane Fuel Cells

National Science Foundation – Research Experience for Undergraduates

Virginia Polytechnic Institute and State University

Abstract

Disulfonated random and multi-block copolymers based on poly(arylene ether sulfone) have been shown to be attractive candidates for fuel cell proton exchange membranes via lab-scale solvent-casting methods. Thus the effects on the PEM final properties were investigated for commercial production using a homemade batch convection drying apparatus that simulates industrial solvent-casting conditions. A random copolymer (BPSH-35) and a multi-block copolymer (BPSH-BPS) of two different sequence lengths (5k and 15k) were investigated. Despite similar ion exchange capacities, the block copolymers with the longer sequence length demonstrated superior proton conductivity, due to a hypothesized phase separation between sulfonated and non-sulfonated segments and a well defined co-continuous microstructure. No considerable effects of the solvent-casting conditions on the properties of the random copolymer were observed, while variations in the properties of the multi-block copolymer films were induced by the use of different solvents. DMAC, with a higher selectivity for the non-sulfonated segments than NMP, produced films with higher proton conductivities.

Ink-jet Printed Cellulose Nanocrystal Substrates for Cell Micropatterning

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Abstract

Cellulose has been used to treat and heal burned skin, sutures, and chronic ulcers. Thus far, microbial cellulose has been researched for such biomedical applications. Instead of using microbial cellulose, our group explored the possibilities of using cellulose from wood pulp. Four pattern templates, circle, square, checkered square, and dots, were prepared using CorelDraw™. Cellulose nanocrystals were printed onto glass slides using ink-jet technology and were used as substrates for cell micropatterning. Mouse brain endothelial cells were incubated for seven days and passed onto culture dishes containing the substrates to test whether cellulose promoted or inhibited cell attachment and growth. After three days of incubation, the substrates were observed using bright field microscopy and also stained with Calcofluor White Stain and viewed under blue light excitation. When stained, the nuclei of the cells were visibly aligned to the pattern of the nanocrystals for the circle, square, and checkered square patterns. Random orientation of cell growth and attachment was observed on the dot patterned substrate. We concluded that when the cellulose nanocrystal pattern was continuous or had a large enough surface area, the cells preferred to align and orient to the pattern of cellulose. When the patterns were too small, in this case, the dot pattern, the cells did not show any preferential alignment or growth on cellulose. Future studies using continuous and larger patterns of cellulose nanocrystals can be used to guide us in applying wood pulp cellulose in the biomedical field.

Adsorption of Phospholipid Bilayers onto Pullulan-modified Cellulose Surfaces

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Abstract

Phospholipid bilayer adsorption onto regenerated cellulose and pullulan 4-bromocinnamate (P4BC) modified cellulose surfaces was investigated. P4BC with a targeted degree of substitution (DS) of 0.08 was synthesized from pullulan and 4-bromocinnamic acid to yield P4BC with an actual DS value of 0.061 ± 0.002 from UV measurements and 0.058 from ^1H NMR. The adsorption of 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC) vesicles onto regenerated cellulose and P4BC modified cellulose surfaces was studied via surface plasmon resonance (SPR) spectroscopy and quartz crystal microbalance with dissipation (QCM-D). The deduced thicknesses from SPR for DMPC layers were ~ 3.7 nm (bilayer) on regenerated cellulose surfaces and were ~ 2.1 nm (monolayer) on P4BC modified cellulose surfaces. QCM-D results also indicated that the DMPC layers on P4BC modified cellulose surfaces were thinner than on regenerated cellulose surface.

Progress Toward a Highly Fluorinated, Sulfonated Diels-Alder Polyphenylene for Use as a Proton Exchange Membrane in Hydrogen Fuel Cells.

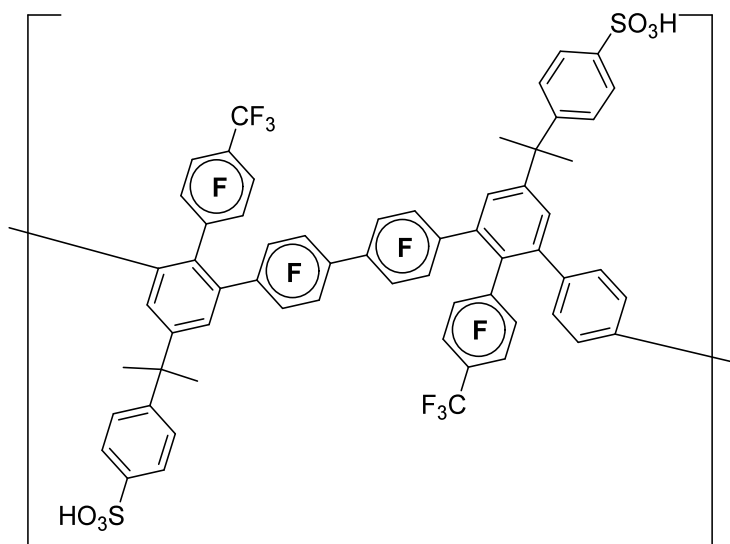
Kelly M. Daly, Jessica P. Evans, and Paul A. Deck*

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Abstract

This paper describes the preparation of two synthetic intermediates along a proposed pathway toward a new class of highly fluorinated, sulfonated polyphenylenes intended for use as proton exchange membrane (PEM) materials in hydrogen fuel cells. The intended polymerization reaction is based on a method developed by Stille in the 1960s, which combines a bis-cyclopentadienone (CPD) monomer with a commercially available diethynylbenzene in a Diels-Alder polycondensation process. The novelty of the present work rests on the high degree of fluorination in our CPD monomers, which is achieved using nucleophilic aromatic substitution chemistry developed in the Deck group over the past ten years. The specific monomer target, 4,4'-bis[1-cumyl-2-oxo-3-(perfluoro-4-tolyl)cyclopentadien-4-yl]octafluorobiphenyl, is based on the previous, successful synthesis of a closely related monomer bearing a *tert*-butyl group instead of the new cumyl group.

Thus, decafluorobiphenyl reacts with (cumylcyclopentadienyl)lithium and sodium hydride in refluxing tetrahydrofuran (THF) to afford 4,4'-bis(1-cumylcyclopentadien-4-yl)octafluorobiphenyl (**3**) in 51 % yield after workup and chromatographic purification. Compound **3** reacts with octafluorotoluene and sodium hydride in THF to afford 4,4'-bis[1-cumyl-3-(perfluoro-4-tolyl)cyclopentadien-4-yl]octafluorobiphenyl (**4**) in 16.3 % yield after purification by silica gel chromatography. Changing the structure of the previously known, analogous intermediates to include a cumyl substituent (intended as a reactive site for post-sulfonation of the proposed polyphenylene) led to interesting technical challenges that are described herein. Also described are the characterization of the two new compounds, which are obtained as inseparable mixtures of regioisomers, by ^1H and ^{19}F NMR spectroscopy.



Dumbbell-Shaped Polysulfones with Hyperbranched Ionic End Groups

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Research on proton exchange membrane fuel cells (PEMFCs) is of high interest, as fuel cells are a promising alternative to current oil usage. PEMFCs are a clean energy source with broad potential applications in transportation vehicles and stationary power. They utilize hydrogen as the fuel and ideally produce water as the only by-product. Proton exchange membranes (PEM) consist of an anode and cathode separated by a polymer electrolyte membrane, with the ideal polymer being stable, long-lasting, and having high proton conductivity. It is imperative that the polymer conduct only protons, as the electrons must pass through an external circuit to create an electrical current. Much of the research in progress is focused on sulfonated aromatic polymers because they possess very high thermal and chemical stabilities and have high proton conductivities. Our approach is to synthesize linear-dendritic ABA copolymers through step-growth polymerization, where A is a hyperbranched polymer with terminal sulfonate groups and B is the linear backbone, in this case poly(ether sulfone) (PES). By concentrating the sulfonic acid groups on the numerous chain ends of the hyperbranched polymers, the ions should cluster together and serve as a channel for proton flow. We have synthesized a monomer for the hyperbranched component, 3,5-bis(4-fluorobenzoyl)phenol, through a previously reported method. Our future research will be directed toward preparing the novel linear-dendritic block copolymers.

**Direct Methanol Fuel Cell Study of a Novel
Poly(arylene ether benzonitrile) and Disulfonated Poly(arylene ether sulfone)
Multiblock Copolymer Membrane**

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Abstract

Direct methanol fuel cell (DMFC) performance and methanol permeability of a novel partially fluorinated poly(arylene ether sulfone) based multiblock copolymer proton exchange membrane was investigated. The multiblock copolymer was synthesized through a nucleophilic aromatic substitution reaction between a phenoxide terminated fully disulfonated poly(arylene ether sulfone) (BPSH100) and a fluorine terminated poly(arylene ether benzonitrile) (6F-PAEB) whose sequence lengths were both 7 kg mol^{-1} . DMFC performance of the multiblock copolymer was similar to a random poly(arylene ether sulfone) based BPSH35 membrane, with a relatively slight decrease in performance at lower cell potentials. Methanol permeability was determined using an open circuit methanol crossover method under live fuel cell test conditions. The 6F-PAEB-BPS100 multiblock copolymer had a low methanol permeability value of $1.617 \times 10^{-6} \text{ cm}^2/\text{s}$.

Influence of magnetic molecules on electron spin scattering in InAs

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Quantum interference between different scattering trajectories of electrons in solid-state systems leads to corrections to the classical electrical resistivity. These corrections result in the phenomena of weak-localization and anti-localization and can be measured in electron transport experiments under applied magnetic fields. The effects present essential and fundamental questions in solid-state physics. Achieving an understanding of the quantum interference corrections leads to significant advances not only in our understanding of the scattering centers which affect the resistivity of solid-state systems but also convey information about the interaction of the electrons with these centers. In particular in the development of advanced electronic systems such as spintronics, a study of the interaction of electrons with isolated spins may lead to new avenues of spin manipulation. Through the use of weak- and anti-localization, we seek to determine the interaction between electrons and the isolated spin systems found in adsorbed magnetic molecules. In particular we focus on InAs films, and study the influence of a monolayer of a magnetic molecule, Mn12, on the spin scattering of the electrons in the InAs accumulation layer. The localization effects were measured at temperatures of 0.4 K. In initial experiments, so far, clear anti-localization is observed but the trends have not yet yielded systematic answers. This situation is likely due to interloping electrostatic effects. We conclude that a system of Mn12 application better suited to the delicate InAs surface is needed.

Development of a Novel Test Fixture to Quantify Mechanically Induced Electrical Shorting of Proton Exchange Membrane for Fuel Cell Applications

Timothy A. Gray¹, NSF REU Student

With input from:

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ABSTRACT

In hydrogen powered fuel cells, the possibility of electrical shorting across the membranes is of potential concern for membrane durability. The significant stack compression stresses could force portions of the gas diffusion layers into the membrane, causing potential gas leakage or electrical shorting sites. Investigating the onset of mechanically induced shorting remains critical to understanding the electrical shorting issue as a whole. In this study, a test fixture capable of quantifying shorting is devised using stackable printed circuit board (PCB) plates with gold contact disks. Samples of membrane electrode assembly (MEA) sandwiched between gas diffusion layers (GDLs) are compressed between PCB plates while current is measured across the contact disks. Success in initial single specimen, ramped load, and tests at room temperature and 60°C suggest that future tests incorporating stacked plates in controlled environments under different loading situations will provide the valuable insights, critical to improving membrane durability with regards to electrical shorting.

Ionic Polymer-Metal Composites as Residual Stress and Humidity Sensors for PEM Fuel Cells

Christopher Horvath, Jacob Davidson, Kahlil Detrich, Dr. Nakhiah C. Goulbourne

Abstract

In this work we research the feasibility of using Ionic Polymer-Metal Composites (IPMC) as sensors for Residual Stress and Humidity within Proton Exchange Membrane (PEM) Fuel Cells. Many methods are currently available for Fuel Cell diagnostics, but each have their own limitations, and as of yet, there is nothing regarding the residual stresses within the PEM. The residual stress within the PEM is a suspected cause of failure in fuel cells, induced by the changing humidity and water production as a result of varying performance. IPMCs are an emerging class of smart materials that can be used for actuation and sensing purposes. As water and Nafion® based smart materials, IPMCs have the potential to serve as sensors within the fuel cell. As a residual stress sensor it would provide another useful diagnostic within fuel cells, and would ideally be for in-situ use. As a humidity sensor it would replace larger apparatuses and possibly be more cost effective.

To investigate the possibility of using the IPMC as a sensor, several tests were performed. Tests were done using an apparatus that holds the IPMC in tension as it dries from a hydrated level to a dry state, while measuring the output voltage and the induced stress from drying. Through a drying test using an input voltage sine function in addition to reading the output voltage it was found that the amplitude of the output voltage shares a linear relationship with the induced residual stress. This was the most significant finding since it shows that with further research, the IPMC shows great promise as a residual stress sensor. A test without the use of an input voltage showed that its output voltage during drying shares no simple relation to the induced residual stress. The tensile properties of the IPMC were also tested using the setup to move a given distance, thus providing an input deformation. This deformation caused an output voltage response at the given point of stress. This shows the IPMC in a different form of sensing than is typical of standard IPMC sensing methods.

Enzymatic Hydrolysis of Cellulose Nanocrystals for Use in Targeted Drug Delivery Systems

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1. Introduction

Thermoplastic and other polymers are used extensively in modern medicine for applications including artificial bone structures, tissue growth scaffolds, and targeted drug delivery systems. Due to their generally benign nature, biocompatibility, and decreased degradation product toxicity, focus has begun to shift to naturally occurring polymers for use in medical applications. Cellulose, the most abundant biopolymer on earth, has demonstrated biocompatibility [1], and mechanical and chemical properties that make it an attractive material for biomedical applications.

Cellulose, a linear glucose homopolymer characterized by $\beta(1,4)$ glycosidic bonds between adjacent glucose molecules (Figure 1), naturally contains both crystalline and amorphous polymer regions, though highly crystalline cellulose fibers are produced by some organisms [2]. Animal and human cells generally lack the cellulase enzymes necessary to digest this polymer. This inability to cleave cellulose chains presents a major challenge to biomedical applications of this material: after performing their function, cellulose molecules must be eliminated by an exogenous mechanism to prevent unnecessary, potentially hazardous, accumulation within tissues. This problem is especially applicable in tissue scaffold and targeted drug delivery applications where *in vivo* cellulose structures must be hydrolyzed without disruption of local cellular function. Our approach to remedy this problem is to administer cellulase enzymes isolated from cellulose digesting organisms as a post-treatment to a cellulose-based therapy to break down the polymer chains to benign, usable glucose molecules after they have served their function in the body. The research presented in this paper focuses primarily on the kinetics and cellular responses to enzymatic degradation of cellulose nanocrystals used for targeted human drug delivery systems, though applications of this research may have much broader uses.

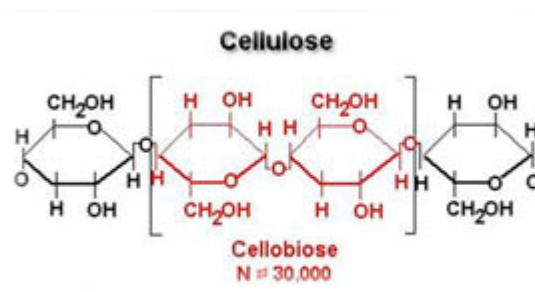


Figure 1. Molecular structure of cellulose [3]

Cellulose nanocrystals are rod shaped cellulose molecules approximately 5 nm in diameter and 100-200 nm long [4] that can be produced biosynthetically by bacteria, such as *Gluconacetobacter xylinus*, or by acid hydrolysis of plant matter. Cellulose nanocrystals are particularly interesting as drug delivery vehicles because of their nearly inexhaustible supply [5], advantageous size relative to cellular structures within the body, the ample availability of side groups available to bind targeting and drug molecules, and their demonstrated biocompatibility [1]. This research explores the potential use of IV administered cellulase enzymes to hydrolyze the $\beta(1,4)$ glycosidic linkages to produce metabolizable glucose *in vivo*.

Two systems for using cellulases to hydrolyze waste cellulose nanocrystals *in vivo* are proposed. First, an extracellular bloodstream system would focus on using cellulases to catalyze hydrolysis of cellulose nanocrystals present in the bloodstream after they have delivered their drugs and been released into the extracellular fluid via cell death. A second, intracellular method would operate by using enzymes that have been endocytosed by the cell to hydrolyze nanocrystals from within the cell prior to cell death, keeping the nanocrystals concentrated only in affected cells. Though both methods are intended to be modified enzyme replacement therapies [6], the second method is intended to be a more direct modification of enzyme replacement therapies for Pompe's disease and other lysosomal storage diseases [7,8] where enzymes are taken up into the cell to perform intracellular catalysis operations.

To determine the future course of action and most appropriate method to study further, three types of experiments were conducted. First, enzymatic hydrolysis kinetics experiments were performed to determine the activity of cellulase on cellulose nanocrystals at human physiological temperature and pH. Kinetic studies of the enzymatic hydrolysis of other forms of cellulose have been performed [9], and several models for intrinsic cellulase kinetics have been proposed. This work will compare the kinetics of nanocrystal hydrolysis to the hydrolysis of other forms of cellulose. Second, cellular viability tests determined if the cellulases caused adverse reactions within cells by addition of cellulase enzymes to the extracellular fluid of cultured mouse brain microvascular endothelial cells (MBMEC) as a model system. Third, a study of cellulase enzyme uptake was conducted with MBMECs to determine if the cells would readily endocytose the cellulase enzymes necessary to catalyze the hydrolysis of waste cellulose nanocrystals from within the cell.

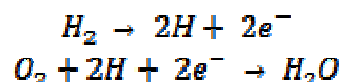
Conductivity of Electrolyte Membranes Within Proton Exchange Membrane Fuel Cells

Craig Keys, Michael Ellis, Chris Cornelius, Patrick Burand

Introduction

Today, renewable energy is critical to the growing demand for power within our country and globally. Fuel cells have been identified as a key enabling technology for the development of more renewable energy systems. These fuel cells can generate power from hydrogen and other fuels such as methanol. Hydrogen is an especially attractive fuel because it can be produced from water and helps reduce dependency on fossil fuels. The idea of a fuel cell was invented in the mid 1800's by Sir William Grove. Many years later, Sir Francis Bacon actually developed the first functional and operational fuel cell. By the mid to late 1950's NASA proceeded with much more concrete research of the fuel cell which was put to use for the Gemini Space Program. The overall concept of this fuel cell technology is that it converts chemical energy into electrical energy which then can be used in a number of ways. There are many types of fuel cells such as phosphoric Acid, direct methanol, alkaline, molten carbonate, and solid oxide but the Proton Exchange Membrane or Polymer Electrolyte Membrane Fuel Cell (PEM Fuel Cell) has gained much popularity for portable and transportation power systems. It is viewed as very promising because of some of its desirable attributes such as their fast startup time, low sensitivity to orientation, and favorable power-to-weight ratio when compared to other types (Energy, 2008 #11). PEM Fuel Cells contain a catalyst layer, gas diffusion layer, a polymer electrolyte membrane, a cathode and anode. This polymer electrolyte membrane is a thin ion conducting membrane which has the unique property of allowing proton transport while blocking the transport of electrons. The fuel (hydrogen) is initially oxidized at the anode by a catalyst (Hill 2006). The most common catalyst is platinum, however it is very expensive. The protons from the oxidation are passed through the electrolyte membrane and the associated electrons are passed through a circuit and used for power production. On the cathode side of the cell, oxygen molecules are introduced to the protons and electrons where the three combine to form product water and heat. Despite its promise, PEMFC technology must overcome a number of hurdles before it becomes commercially viable. Many of these challenges are related to the membrane material. Membranes need to be more conductive at wide ranges of temperatures and relative humidities and need to be more durable. The basic reaction that occurs within the cell is shown in equation 1.

Equation 1: Chemical Reaction of PEM Fuel Cells



Development and Testing of Micro-tubular Fuel Cells for United States Air Force Micro-Aerial Vehicles

Joshua M. Kezele

Abstract

The United States Air Force uses micro-aerial vehicles (MAV) for reconnaissance and damage assessment missions. Presently, the MAVs use a battery that powers the vehicle and its equipment. The battery is only able to provide power for approximately 20 minutes, which is not a suitable amount of time. A bigger battery is not a viable solution because this would increase the weight of the MAV and the weight that a soldier must carry, so a fuel cell system that increases the runtime of the MAV while providing sufficient power without increasing the MAVs weight is desired.

The first fuel cell system was designed by a group of senior Mechanical Engineering students at Virginia Polytechnic Institute and State University. The system did not meet the volume, voltage, current and power requirements, so a new system was designed this summer. Testing of the new system will be completed by a new group of senior engineering students that will also work on improving the performance of the individual fuel cells while exploring the possibility of using a Hydrogen-On-Demand™ device.

Antiproliferative Effect of Various Fruits against Human Breast Cancer Cell Grown in Vitro

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Virginia Polytechnic Institute and State University

INTRODUCTION

Breast cancer is the most common cancer among American women (1). The chance of developing invasive breast cancer at some time in a woman's life is about 1 in 8 and it is the second leading cause of cancer death in women (2). The advances were made in breast cancer treatment but the side effects are still undesirable to the patients. Therefore, complementary or alternative medicine is required to help relieve symptoms, ease treatment side effects, and improve quality of life.

There is increasing interest in the role of nutrition and specific dietary constituents in the prevention of cancer. Recent publications show various constituents of fruits to be beneficial in protecting cells from different forms of cancer (3). Fruits are rich sources of antioxidants. Fruits, especially in berries, contain great amount of phenolic compounds such as anthocyanin, ellagitannins and ellagic acid (6). These polyphenolics are capable of scavenging oxygenated free radicals which can damage cellular components such as DNA, proteins, or membrane lipids (4). In addition to their antioxidant properties and ability to protect cellular components from oxidative stress, polyphenolics may have potential benefits towards reducing the risk of cardiovascular diseases and cancers by suppressing cancer proliferation, angiogenesis, and inducing cancer cell apoptosis (7). In earlier cell culture studies, polyphenolic extracts from various fruits have been shown inhibitory effects towards cancer cell growth but there is no information about how they affected on the normal cell.

Therefore, the objective of this study was to screen all the fruit, vegetable, and Chinese traditional herb extracts in our laboratory to determine how they affect breast cancer cell as well as normal breast cell at different concentration of sample extracts. By comparing their antiproliferative effectiveness against both breast cancer cell and normal cell, the best bioactive candidate for breast cancer cell will be determined.

Solvent Mass Uptake Studies of Biphenyl Poly(Arylene Ether Sulfone) Copolymer Thin Films via Quartz Crystal Microbalance with Dissipation Monitoring

Erin Littleton, Abdulaziz Kaya, and Alan R. Esker

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Abstract

The swelling behavior of thin films of the potassium salt (BPS-35) and acid (BPSH-35) forms of biphenyl poly(arylene ether sulfone) copolymers containing 35 mol% sulfonation are analyzed in order to determine solvent uptake within materials that have potential applications as proton exchange membranes (PEM) in fuel cells. Using a quartz crystal microbalance with dissipation monitoring (QCM-D), the change in mass of the polymer films are tested in common fuel cell solvents: water, methanol, ethanol, and isopropanol. It was determined that dissipation values do not correlate with the thickness of the polymer films; however, mass uptake decreases with increasing film thickness. Both BPS-35 and BPSH-35 thin films exhibited elevated degrees of solvent uptake in methanol compared to those in water. Ethanol and isopropanol data yielded results that were more difficult to interpret because greater swelling may weaken the assumption that the film can be treated as a rigid extension of the quartz crystal.

MANIPULATION OF THE NANOSTRUCTURE OF AN IONIC POLYMER METAL COMPOSITE VIA POST-POLYMERIZATION SULFONATION OF THE IONOMER MEMBRANE

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Introduction

An ionic polymer metal composite (IPMC) is composed of a thin layer of ion-containing polymer membrane material electroplated on both sides with a noble metal. IPMCs are sensors and are of great interest to the scientific community because of their ability to produce large bend motions upon electric stimulus. These electro-active polymers have the mechanical properties to have the potential to be used in applications such as biomedical devices, artificial muscles, and robotics.

Much of the current research done with IPMCs use the perfluorosulfonate class as the ionomer membrane. Nafion is composed of hydrophobic backbones that cluster into a semi-crystalline matrix and side chains with attached sulfonic groups that aggregate into water filled clusters¹. James has developed a scheme for the diagram of ionic aggregates and observed small clusters 2-5 nm in diameter gathering into large framework up to 30 nm in diameter. The counterions added to the membrane are attracted to the fixed aggregates which encapsulate the water molecules². After applying potential energy, the cations migrate to the cathode, and the water diffusion occurs simultaneously due to water salvation-shell migration.

Wu and his constituents have used multiple techniques to study the physical, electrical, and mechanical properties of Nafion. Now that the basics have been established research points towards to underlying nano-scale manipulations that may be superimposed on the Nafion membrane, but due to Nafion's complex nature research is limited. Disadvantages with current IPMCs such as manufacturing costs, force output, scalability, and inconsistency in processing are inhibiting the electroactive polymer material for use in real world applications³.

Instead of trying to alter the Nafion based IPMC, in this study sulfonated Syndiotactic polystyrene (SsPS) was used as the ionomer membrane within an IPMC. In 2005, Phillips explored other classes of polymers that have the ability to act as actuators, yet for lack of structured ionic morphology, the sulfonated ethylene vinyl alcohol displayed slower actuation kinetics⁴. Nafion is currently the benchmark ionomer membrane investigated in IPMCs. However, due to the high cost of the ionomer and significant challenges in synthesis and processibility, other ionomers should be investigated as substitutes. SsPS has been used as a model semi-crystalline ionomer to study the effect of sulfonation on crystallization and kinetics. Due to the wealth of fundamental information available between sulfonation and crystallinity, SsPS may be a prime candidate as an ionomer membrane in IPMCs⁵.

We propose a novel sulfonation procedure to prepare SsPS. Previous investigations of SsPS have focused on sulfonating SPS while in solution state leading to a random ionomer⁵. Sulfonating in the gel state will prohibit the bulky sulfonating reagent complex from entering the crystalline domains present. Solution state sulfonation

above two mole percent has shown to significantly decrease crystallinity. This presents a challenge in IPMC actuation because sulfonation less than two mole percent is not ideal for optimum water uptake affecting actuation.

The purpose of this study was to increase the mechanical properties of styrene derivatives as ionomers in IPMCs. We have quantified the tip displacements and rates of our novel SsPS based IPMCs. Through DSC, we have investigated the differences in crystallization kinetics between gel and solution state sulfonated sPS. Sulfonating sPS in the gel state may yield a potential route to provide higher degrees of sulfonation while maintain the ability to crystallize. This aspect of controlling the crystallinity of Syndiotactic polystyrene is beneficial from fundamental and applied aspects in IPMCs³.

Blister Testing: Correlating Pressure and Displacement Data to Determine Biaxial Stress States on Gore® 57 Membrane for Hydrogen Fuel Cells

Emily Mieritz, Jake Grohs, and Scott Case

Proton Exchange Membranes (PEM) are a vital component of hydrogen fuel cells. Their mechanical properties need to be quantified in order to better understand the lifetime and durability of fuel cells. One such property, the biaxial burst strength of the membrane, can be quantified by means of the blister test. Blister tests pressurize a circular plane of membrane until failure; just like blowing a bubble. Ultimately, fuel cells have to meet U.S. automotive standards in order to be competitive. As of 2007, the President's Hydrogen Fuel Initiative reports 1350-hr durability, or about 40,000 miles capability. Its goal for 2015 is 5000-hr durability. [1]

The DIC ARAMIS® will be used to measure membrane deformation. It has been tested in multiple settings which required high accuracy, such as a study of how moving tires deform under different loads. Deformation of the tires tested was measured with accuracy in millimeters. Another example of ARAMIS' reliability is that it was able to process data from a camera with a frame rate of 30,000 per second. The object was a screw coming through a metal plate, and it took only about 1.5 ms. ARAMIS was able to calculate the major strain of 7% on the sample plate [2]. Hopefully, the DIC will be able to calculate the displacement of the membranes with similar accuracy.

The membranes to be tested are Gore-Select® Series 57 and DuPont's Nafion. The tests will be run at 90° C, near fuel cell operation temperature, and above a transition temperature of roughly 70° C, which makes it more able to stretch than at room temperature. The higher temperature causes an accelerated degradation condition, simulating a longer test at a lower temperature. [3]

The deformation measurements can describe the stresses on the membrane through the following simplified Hencky's solution for a pressurized circular membrane:

$$1) \quad w = a \left(\frac{pa}{Eh} \right)^{1/3} \left\{ \sum_0^n A_n \right\} \quad (1) \quad [4]$$

$$2) \quad \sigma_r = \sigma_\theta = \frac{B_0}{4} \left(\frac{Ep^2 a^2}{h^2} \right)^{1/3} \quad (2) \quad [3]$$

where w is the deformation of the blister at the center and σ is the stress at the center. B_0 is estimated to be 1.777, based on Poisson's ratio [3]. A_n is a constant dependent on B_0 . Membrane thickness, h , blister radius, a , the pressure on the sample, p , and the temperature at which the test was run, are assumed to be constant throughout the trial. The modulus of Elasticity, E , will be estimated in the first equation and used to estimate the UTS using the second.

Synthesis and Characterization of a Novel Class of PEG Ionenes with Varying PEG Lengths

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ABSTRACT:

Polycation-mediated gene transfection is a method for the treatment of genetic diseases and cancers. Polyionenes are an ideal class of materials for studying the structure-property relationships of polycations for gene transfection. A family of polyionenes containing polyethylene glycol (PEG) segments in the main chain and *boc*-protected amine groups were successfully synthesized. PEG was introduced into the main chain in order to reduce cytotoxicity. The molecular weights of the PEG chains were systematically varied to study the effect of charge density on transfection behavior. *Boc*-protection enabled the charge density to be further varied without changing molecular weight, and it also enabled an investigation of effects of protonatable secondary amine in the polyionene chain on transfection behavior. Thermal characterization showed a two-step degradation of the polymers, with the amine segments degrading first. Crystallization behavior was observed for most of the ionene chains, with the T_c increasing as the PEG segment length was increased. T_c also increased with deprotection. Further studies will be required to fully characterize and understand this behavior.

Electrochromic Devices by Ionic Self-assembled Multilayers (ISAMs).

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Electrochromic (EC) devices exhibit a reversible change in color, absorbance and transmittance when an outside voltage source is applied to the conductive substrate. Conducting polymeric EC devices have several present and potential applications due to their combined capacities for fast switching-speeds with high contrast. They are particularly being considered for technologies such as smart windows and flat panel displays because EC devices require minimal power consumption. Our present work with ionic self-assembled multilayer electrochromic devices were assembled on glass slides coated with indium tin oxide as our substrate, poly(allylamine hydrochloride) (PAH) as the cationic polymer at a concentration of 10 mM and pH 3.5, and copper phthalocyanine (CuPhth) as the anionic conductor. A second multilayer set under investigation was comprised of PAH and a water soluble anionic polythiophene dye, sodium poly[2-(3-thienyl)ethyloxy-4-butanedisulfonate] (PTEBS). Multilayer films of the two sets of materials ranging from 5-120 bilayers were fabricated and the film thickness and absorbance were measured from 300-1100 nm. The PAH/CuPhth films exhibited a linear increase in film thickness and absorbance with the number of bilayers and the ITO slides exhibited a change of color from royal blue to purple upon voltage application between 0.6 and 1.0 V. The PAH/PTEBS materials showed an exponential increase in film thickness and absorbance versus the number of bilayers.

Cloning of Alpha-synuclein and Firefly Luciferase Fusion Constructs

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Abstract

Approximately six million people worldwide are affected with Parkinson's Disease. This is just one example of several neurodegenerative diseases that rob individuals of control over muscle movement. The pathological hallmark of neurodegenerative diseases is the presence of protein aggregates, known as Lewy bodies. Current therapies are ineffective, as they are purely symptomatic. They return some quality of life, yet in essence merely prolong the progression of the disease. These therapies focus on finding small molecules targeted at the DNA and protein levels. The goal was to create a recombinant DNA fusion molecule that coded for the neurotoxic protein, alpha-synuclein. Then, using *in vitro* transcription, the mRNA developed will be used to find small molecular inhibitors of alpha-synuclein's translation. By inhibiting the synthesis of this protein, its contribution to Lewy bodies is minimized, and the progression of the disease can be halted.

Flame Synthesized Carbon Nanostructures as Anodes in Microbial Fuel Cells

Abstract

Microbial fuel cells (MFC) are a viable renewable energy option, especially in their potential to collect electricity produced by bacteria in wastewater treatment facilities. Chemical mediators have been used in the past to facilitate electron transfer from the bacteria to the anode, but our microbial fuel cells use carbon nanostructure coated stainless steel mesh, a novel anode material hypothesized to increase direct transfer from the bacteria to the anode. The nano-scale surface characteristics are three orders of magnitude smaller than the dimensions of the bacteria. A microbial fuel cell experiment was run with a mixed culture of anaerobic bacteria. Four cells were set up, two with stainless steel mesh anodes and two with carbon nanostructure coated anodes. The two cells with carbon nanostructures performed better and one CNS anode showed growth of bio-like structures on it when viewed under low-vacuum mode in the Environmental Scanning Electron Microscope. Cell 3 with a CNS-coated anode produced the maximum amount of current of 115 microAmps. These bio-like structures on the CNS anode could mean that the bacteria are more prone to attach to the CNS than a plain stainless steel substrate, thereby facilitating direct electron transport and eliminating the need for expensive chemical mediators. An investigation into the durability of carbon nanostructures subjected to water flow was also conducted, along with a comparison between CNS deposits on plain stainless steel mesh substrates and substrates coated with ferrofluid and then CNS deposited. The results were that CNS showed better attachment to the plain stainless steel mesh substrates than those coated with ferrofluid, and a significant amount of carbon still remained on those substrates after water flow (44 at%). This supported the decision to use plain stainless steel substrates with CNS in the microbial fuel cells instead of those coated with ferrofluid first.

Synthesis and Characterization of a Rhodamine Labeled Peptide for the Assay of Pin1 Inhibitors

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Abstract- Pin1 is an enzyme 163 amino acids long that catalyzes the *cis/trans* isomerization of peptides containing specific pThr/pSer-Pro motifs. Pin1 has been shown to be overexpressed in many cancers such as breast, lung, and brain which could be due to its effect on different cellular pathways.¹ It has been determined that a peptide corresponding to the human Cdc25c-T48 phosphatase has high binding affinity to the full length Pin1.² The goal of this research was to design an assay utilizing a substrate based on the specific binding sequence VPRpTVP in the Cdc25c with an aromatic rhodamine label on the n-terminus, Pin1, and specific binding/catalytic inhibitors. The rhodamine label provides qualitative observation of the ligands that do not present affinity for Pin1 in the WW domain through fluorescence.

Characterization of the Membrane Material Found in Proton Exchange Membrane Fuel Cells (PEMFCs)

Duane Rollins and R. L. West, Virginia Tech

Summary

The membrane material found in proton exchange membrane fuel cells (PEMFC) is under a biaxial state of stress when the fuel cell is in operation. Blister testing is used to represent this state of stress in the membrane. I based my virtual model in ABAQUS on the experimental setup of the blister tests. Many different models were used to verify the data such as elastic and plastic axisymmetric models, a 3D cube model, and a full 3D plasticity model of the testing. Since a virtual model is only a representation of the dominant mechanics many assumptions were made such as the interaction of the nut on the Teflon washer or the interaction of the membrane on the pressure vessel. Both were assumed to behave as if they were glued together. To reduce processing time, a quarter model of the full 3D model with plasticity was used. Once the model began to produce reasonable data, those results were converged by varying the stability factor, changing the number of elements, and using reduced integration. Strain and displacements are the two quantities that can be directly compared from the experimental setup to the virtual model. From the virtual model, the maximum displacement was found to be 5 mm compared to the experimental data which showed a maximum displacement of 15 mm at 16 kPa. The discrepancies in the maximum displacement are due to many reasons two of which are that the temperature dependence data and rate dependence data were not added to the virtual model. The addition of those factors would provide better results and is a way to continue this research in the future.

Production of Metallic Flavor Compounds by Oxidation of Oral Cell Membrane Fatty Acids and its Prevention by Antioxidants and Chelating Agents

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Virginia Tech, Blacksburg, Virginia August 8, 2008

Abstract:

Unpleasant metallic flavors from drinking water and food can cause consumer complaints and become an issue for the water and food industry. Iron found in food and water can catalyze the oxidation of fatty acids commonly found in the oral epithelial cell membranes. This process produces carbonyls that give off a metallic flavor. Metallic off-flavor is also an issue for the people affected with certain diseases including cancer and taking certain medications and may affect their healing and nutrition. This study examined the oxidation of selected fatty acids (arachidonic, linoleic, oleic, and palmitic) in the presence of ferrous iron and several antioxidants and chelating agents. Solid phase microextraction, 2,4-dinitrophenylhydrazine derivatization, and thiobarbituric acid reactive substances analysis were used to determine the carbonyls produced and the extent of lipid oxidation. Several aldehydes, ketones, alkanes, and alcohols were detected in the headspace of the samples reacted with iron. The most efficient oxidation prevention compound is determined as EDTA, although vitamin E also showed the potential to have inhibitory effects as well. The findings may be used to determine a method to prevent oxidation and hence the metallic flavor in the mouth which would greatly benefit the people suffering from the chronic off-flavor in their daily food and beverage consumption.

Key words: Metallic flavor, lipid oxidation, iron, SPME, TBARS, DNPH, antioxidants, chelating agents

GELATIN AND ALBUMIN MICROSPHERES FOR DRUG DELIVERY IN BONE REGENERATION

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INTRODUCTION: Hundreds of irregular and underdeveloped bone growth cases occur each year, and these conditions often leave vital organs exposed. Bone tissue engineering through drug delivery offers a means to regenerate growth in these areas. Since April 2000, the FDA has certified microsphere drug carriers targeted to tumors for cancer patients. **METHODS:** Previous studies have reported gelatin microspheres that were fabricated by crosslinking them with glutaraldehyde in an water-in-oil emulsion. We adapted this method and extended the investigation to include albumin, which is a significantly more complex protein. A series of alternative, non-toxic reducing sugars were investigated as crosslinking agents to replace glutaraldehyde in these microsphere formation reactions using both gelatin and albumin as the matrix proteins. Glucose, fructose, and D-ribose were examined in systematically varied increments. **RESULTS:** In vitro testing with gelatin hydrogels indicated that glucose and fructose were not viable alternatives, but stable microspheres were produced with D-ribose. Albumin microspheres were successfully fabricated with two different crosslinking reagents: glutaraldehyde and D-ribose. Various concentrations of D-ribose were investigated to improve the mechanical integrity of the new albumin microspheres, and it was found that microsphere aggregation decreased with increasing amounts of the reagent. The percent of crosslinking in the microspheres was determined through a trinitrobenzenesulfonic acid (TNBSA) assay. **CONCLUSION:** Albumin microspheres were fabricated and characterized successfully. Further work will focus on optimizing microsphere size and size distribution.

Formation of Magnetite Clusters using a Confined Impinging Jet Mixer

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Superparamagnetic nanoparticles (SPM NP) are commonly employed as magnetic resonance imaging contrast agents. Magnetite (Fe_3O_4) is of increasing interest because of its high magnetic susceptibility in an applied magnetic field. It has been shown in the literature that an increase in size of transverse NMR relaxivity agents leads to a significant decrease in T2 relaxation times and thus higher contrast in an MRI. It is therefore important to develop methods and conditions for controlling the size of polymer-stabilized magnetite clusters. Our strategy is to elucidate critical coagulation concentrations of water for magnetite particles that have been coated with an amphiphilic poly(propylene oxide-*b*-ethylene oxide)-OH (PPO-*b*-PEO) copolymer to control clustering size through the use of a confined impinging jet (CIJ) mixer. Using the critical coagulation concentrations, operating conditions for the CIJ mixer have been found where micellization of the copolymer occurs simultaneously with magnetite clustering. Preliminary results have shown that control over the size distribution may be possible by changing the concentration of water in the mixing chamber.

Coefficient of hygral expansion for NR-211

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Abstract

The coefficient of hygral expansion (CHE) is a parameter needed to run a fuel cell stress prediction model. This study summarizes the published literature for sorption and strain properties of Nafion and gives preliminary results from experimental determination of CHE for NR-211. Although no literature directly reported the CHE of Nafion, many articles covered sorption characteristics and their influence on mechanical properties. The knowledge gained in the literature survey was used to determine experimental parameters such as equilibration time. The CHE was determined experimentally at 80 °C by hanging a sample of NR-211 in a humidified environment and stepping the humidity from 45% to 65 % to 45% relative humidity (RH) in increments of 5% RH. Each humidity level was held for 2 hours. The CHE determined from these tests was 1.14%.