Energy Storage and Distributed Energy Generation Project

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INTRODUCTION

This report serves as the Final Report and deliverable under the “Energy Storage and Distribution Energy Generation Project” carried out by the Transportation Energy Center (TEC) at the University of Michigan (UM). An interdisciplinary research team has been working on fundamental and applied research on:

- distributed power generation and microgrids,
- power electronics, and
- advanced energy storage.

The long-term objective of the project was to provide a framework for identifying fundamental research solutions to technology challenges of transmission and distribution, with special emphasis on distributed power generation, energy storage, control methodologies, and power electronics for microgrids, and to develop enabling technologies for novel energy storage and harvesting concepts that can be simulated, tested, and scaled up to provide relief for both underserved and overstressed portions of the Nation’s grid. TEC’s research is closely associated with Sections 5.0 and 6.0 of the DOE “Five-year Program Plan for FY2008 to FY2012 for Electric Transmission and Distribution Programs, August 2006.”

The progress report submitted in December 2006 contained a series of white papers, describing the following potential research topics:

- 1) Photo-Assisted Catalytic Carbon Steam Gasification to Syngas for Distributed Power Generation
- 2) Formulation of Novel Materials for Hydrogen Separation
- 3) Grid Applications for Novel Energy Storage
- 4) Advanced Thermal Management of Lithium Ion Battery System for Grid Energy Storage Applications
- 5) Control and Communications Requirements of Grid Connected Fuel Cells
- 6) Modeling and Thermal Management of Vehicle Fuel Cell System for Power Supply into Micro-grid
- 7) High Temperature High Power Density Silicon Carbide Converter for Renewable Energy System and Power Grid Applications
- 8) Novel Concepts for Chemical Energy Harvesting and Chemical to Electric Energy Conversion
- 9) Low-Cost, Nanostructured Proton Exchange Membrane Fuel Cells

In meetings in Washington, D.C. with Gil Bindewald of the DoE Office of Electricity Delivery and Energy Reliability, and with Assistant Secretary of Energy Kevin Kolevar, it was agreed to consolidate the various topics outlined in the December 2006 progress report into a unifying theme, namely the development of enabling technology that allows for energy self-sufficient farms as an example for compact, distributed energy systems.

The basic idea behind the energy-self-sufficient farm concept is that biomass utilization could possibly be more efficient by developing small-scale, distributed technologies for gasifying locally-available feedstocks. A major challenge for such distributed biogas systems is that they must be flexible enough to operate with feedstocks of widely varying composition in a steam/oxygen gasifier. The hydrogen-rich gas produced in these feedstock-flexible gasifiers can be directly used as fuel for heating, steam production, and crop drying. The gasifier output can also be blended with digester methane from animal waste or landfills for use as a fuel for internal combustion engines, or processed into syngas suitable for solid oxide fuel cells to generate electricity onsite.

The gasifier output can be passed through a downstream fuel processing unit, to generate a relatively pure mixtures of syngas suitable for powering solid oxide fuel cells (SOFC) for distributed electricity generation. This syngas can also serve as feedstock for advanced Fischer-Tropsch synthesis, providing for the conversion of biomass into alcohol or liquid transportation fuels. The ultimate fully-integrated and self-sufficient bioenergy system could have wide ranging applications ranging from farms to military bases to remote locations with limited access to the electric grid.

The following sections of the Final Report discuss the results of our research efforts supporting the long-term goal of enabling technologies for energy-self-sufficient farms.

RESEARCH AREA 1

SYNGAS (CO+H₂) PRODUCTION FROM FUEL-FLEXIBLE BIOMASS GASIFIER

PIs: Prof. Johannes Schwank and Dr. Andy Tadd
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The specific objectives were:

- To develop, design, construct and operate a prototype modular reforming reactor configuration capable of converting gasifier product streams of varying composition into SOFC-quality syngas.
- To develop a conceptual design of a small-scale, compact, modular reactor system integrating the reforming reactor with upstream components capable of converting feedstocks from a wide variety of locally-accessible sources (e.g., lignitic and brown coals, peat, wood, purpose-grown energy crops, solid waste, agricultural waste, and animal waste) into a relatively clean product stream containing combustible gases with condensables as minor products.

This project, with additional funding provided by DoE-NETL through a University of Michigan subcontract with NextEnergy in Detroit, Michigan, will demonstrate the production of SOFC-quality syngas produced on site from locally available mixtures of feedstocks. The *total* technology demonstration program, containing an integrated gasifier and reformer system (Figure 1), will require a sustained research and development effort over approximately five years, with resource requirements in the range of \$8 - 10 million. Ultimately, it is envisioned that the technology that is developed would be transferred to industry, serving as key components of a self-sufficient distributed electricity generation system that could be used on farms, in remote populated areas, military bases and combat zones.

Syngas is typically made by gasifying carbonaceous feedstocks in air and consists of a mixture of carbon monoxide and hydrogen that often contains high levels of nitrogen. A higher-BTU product can be produced by using oxygen and/or steam as the oxidizer in the gasification process. Syngas produced with air has a combustion energy of about 130-150 BTU/ft³. Steam/oxygen gasification methods can produce a variety of gases extending from carbon monoxide (CO) and hydrogen (H₂) mixtures at 250-300 BTU/ft³ to a range of synthetic natural gas (SNG) products with combustion energies in the 950-1000 BTU/ft³ range.

Mixtures of CO and H₂ are sometimes used directly as a fuel gas, although at lower BTU levels supplementary fuel is typically required to maintain stable combustion and to minimize combustion emissions. Alternatively, most of the CO can be removed by reacting the gas with steam using the so-called water gas shift reaction $[(\text{CO} + \text{H}_2) + \text{H}_2\text{O} \rightarrow \text{CO}_2 + 2\text{H}_2]$, followed by CO₂-stripping using the Sulfinol process or equivalent. The result is relatively pure hydrogen that may be suitable for use in hydrogenation processes or in SOFCs or, after further refining to at least “five 9s” grade, for PEM fuel cells.

Figure 1: Conceptual sketch of self-sufficient bioenergy system

SOFCs are highly efficient direct generators of electricity that are operated at high temperatures¹. They can be operated with syngas, mixtures of CO and H₂ and have more tolerance for contaminants, such as sulfur². An attractive feature of SOFCs is that they produce not only electricity, but also high temperature waste heat, whereas most other fuel cell types produce electricity and low temperature waste heat. The residual fuel and high temperature waste heat can be used in bottoming cycles such as gas turbines, or as a heat source for fuel reforming. Thus, as a total system, SOFCs can achieve higher efficiency than low-temperature fuel cells.³ The state-of-the-art SOFC reformers can handle natural gas, gasoline and diesel fuels, but impurities in the fuels can cause catastrophic failures due to deactivation of the catalysts in the fuel cell.

Due to their high temperature of operation, SOFCs can operate on syngas (a mixture of carbon monoxide and hydrogen) produced from natural gas, liquid transportation fuels or solid fuels such as coal or biomass. To date, the majority of syngas for SOFCs has been generated by reforming natural gas, which is a relatively mature technology. Fuel reforming of natural gas can take place in three different ways: external reforming in separate reactor systems, indirect internal reforming, where the reformer is thermally coupled to the SOFC, and direct internal reforming, where the anode of the SOFC also serves as reforming catalyst. In all cases, sulfur compounds

¹ Sandrine Colson-Inam, Solid Oxide Fuel Cells-Ready to Market?, Fuel Cell Today, January 7, 2004.

² James Zizelman, Steven Shaffer and Subhasish Mukerjee, Solid Oxide Fuel Cell Auxiliary Power Unit-A Development Update, SAE Technical Paper Series, March 4-7, 2002.

³ X. Ma, L. Sun, C. Song, A new approach to deep desulfurization of gasoline, diesel fuel and jet fuel by selective adsorption for ultra-clean fuels and for fuel cell applications, Catal. Today 77 (2002) 107-116

must be removed prior to fuel reforming. The high sulfur levels typically encountered in syngas derived from fossil sources or biomass (>100ppm) would result in irreversible performance loss. One of the reasons for this phenomenon is that at these high levels, sulfur penetrates into the electrolyte and poisons it.

There is a great deal of ongoing effort in fuel processing to produce hydrogen from various primary fuels via steam reforming, partial oxidation, or autothermal reforming^{4,5,6,7,8,9}. At the University of Michigan (UM), a DoE-funded project led to the development of a prototype compact gasoline reformer¹⁰. More recently, this work has been extended with funding from the U.S. Army into development of compact reformers for kerosene-based fuels, undertaken by UM's Transportation Energy Center (TEC). A groundbreaking insight gained in this research is that reforming of hydrocarbon mixtures is much more complex than dealing with individual components¹¹. In mixtures, synergistic effects start to appear, which lead to changes in chemical mechanisms and thus influence the quality of the reformat. The non-linear behavior of hydrocarbon mixtures provides a complexity that investigations of single component model compounds are not able to properly capture.

The complexities involved in generating SOFC-grade syngas have important ramifications for utilization of either coals or biomass as a feedstock. For example, a DOE study examined the composition of gasifier products obtained from three different sources of biomass, poplar, switch grass, and mixed wood (Table 1).¹² The results show that in addition to the expected mixture of H₂, CO, and CO₂, a variety of other chemical species is formed, including methane, ethylene, benzene, and toluene. Furthermore, varying amounts of H₂S and NH₃ are formed. The relative amounts of the products depend on the biomass type. Most notably, the H₂S concentration in switch grass is well beyond the sulfur tolerance limits of SOFCs, and switch grass leads to large amounts of cyanide formation.

If coal feedstocks alone are used, the results are similar but present different challenges. Gasification of coal under similar conditions using oxygen-steam mixtures (often called "hydrogasification") produces a somewhat similar gas (see the first column

⁴ X. Wang, R. J. Gorte, A study of steam reforming of hydrocarbon fuels on Pd/ceria, *Appl. Catal. A: Gen.* 224 (2002) 209-218.

⁵ J. Lampert, Selective catalytic oxidation: a new catalytic approach to the desulfurization of natural gas and liquid petroleum gas for fuel reformer applications, *J. of Power Sources* 131 (2004) 27-34.

⁶ Q. Ming, T. Healey, L. Allen, P. Irving, Steam reforming of hydrocarbon fuels, *Catal. Today* 77 (2002) 51-64.

⁷ L. J. Pettersson, R. Westerholm, State of the art of multi-fuel reformers for fuel cell vehicles: problem identification and research needs, *Int. J. of Hydrogen Energy* 26 (2001), 243-264.

⁸ C. Song, Fuel processing for low-temperature and high-temperature fuel cells challenges, and opportunities for sustainable development in the 21st century, *Catal. Today* 77 (2002) 17-49.

⁹ T. Luo, J. M. Vohs, and R. J. Gorte, An examination of Sulfur Poisoning on Pd/Ceria Catalysts, *J. of Catalysis* 210 (2002) 397-404.

¹⁰ "Fuel Processor for PEM Fuel Cells", DoE Contract DE-FC04-02AL67630

¹¹ Gould, Benjamin D.; Tadd, Andrew R.; Schwank, Johannes W.. "Nickel-catalyzed autothermal reforming of jet fuel surrogates: n-Dodecane, tetralin, and their mixture", *Journal of Power Sources*, **164**(1), (2007) 344-350.

¹² Richard Bain, "Biomass Gasification Overview", January 28, 2004, NREL; see also <http://www.msenergy.ms/Gasification%20-%20Mississippi%20Presentation%20v2.pdf>

in Table 1). Of course, coals vary widely and thus the gas composition also varies widely. Although no data are shown here, coals can also result in high benzene, toluene, ammonia and cyanide levels.

None of these four gasifier product streams would be suitable as direct feed for an SOFC, because of the presence of sulfur and nitrogen containing contaminants, as well as benzene and toluene. And, it is reasonable to expect that other types of feedstocks would lead to similar, unsuitable gasifier product streams. Converting each of these three gasifier product streams into SOFC-grade syngas would require the development of feedstock-specific reforming methods. This is certainly an option for large-scale facilities, where the process can be optimized for one specific feedstock. But for distributed generation of electricity on a smaller scale, it would be much more advantageous to make use of mixtures of locally available flexible feedstocks, such as peat, agricultural waste, corn stover, wood products, etc. In such a case, the gasifier product stream would vary considerably depending on whatever feedstock type is available at a given location or time. Consequently, the downstream processing unit that makes SOFC-grade syngas must be able to accommodate fluctuations in the composition of the gasifier output. This represents a major challenge for the design of a fuel processing system downstream of such a gasifier.

<i>Table 1: Typical Gas Yields from Biomass and Coal</i>				
Feedstock Type	Typical Midwestern Coal	Hybrid poplar	Switch grass	Mixed Woods
H ₂ , vol %	22.8	33.99	24.31	31.82
CO	18.0	36.67	39.47	31.59
CO ₂	18.5	17.91	14.97	17.96
CH ₄	14.1	12.56	13.77	11.73
C ₂ H ₄	0.5 (as C ₂ H ₆)	4.41	5.86	4.50
Benzene	NA	1.35	0.96	1.06
Toluene	NA	0.31	0.20	0.24
H ₂ /CO	1.27	0.93	0.62	1.01
H ₂ S, ppmv	9,000	64-72	323-396	36-63
Ammonia, ppmv	Always present	290 max	760 max	339-369
Cl ⁻ cond, ppm-m/v	NA	0	486 max	4 max
K ⁺ cond, ppm-m/v	NA	10 max	208 max	7 max
Tot org. C cond ppm-m/v	NA	2060 max	2320 max	2480 max
Cyanide, ppm-m/v	Always present	37	1442-1472	ND

Table adapted from:
Richard Bain, "Biomass Gasification Overview", January 28, 2004, NREL

We have undertaken work on the conceptual design of a fuel flexible reformer system for biomass derived gas. Since the design of the reformer unit critically depends on the steady-state and transient performance of upstream gasifier units, a

comprehensive survey of the existing scientific literature on carbonaceous feedstock gasification has been conducted, along with an assessment of the mechanistic aspects of feedstock gasification, with emphasis on the effect of feedstock type, blend and reaction conditions on product composition. Special attention has been paid to the details of heteroatom chemistry and the mechanistic aspects of tar formation. Figure 2

Figure 2

Schematics of feedstock-flexible reformer unit.

provides schematics of the feedstock-flexible reformer unit designed under this program.

Current gasifier units are based on several different reactor configurations, including but not limited to updraft gasifiers, downdraft gasifiers, fluid-bed gasifiers, circulating fluid-bed gasifiers, and entrained flow gasifiers. Each of these reactor types has its own technical challenges regarding feed pretreatment, feeder reliability, and heat integration. A critical question is which of these reactor technologies lends itself best for scaling down to the small, compact size required for this project.

We have initiated experiments to investigate the thermal decomposition of various types of biomass, using thermogravimetric analysis coupled with infrared spectroscopic analysis of the evolved gases. For calibration purposes, the thermal decomposition of key biomass components, including lignin, cellulose, and hemicellulose has been carried out. The results of these studies provide important insights and data for specifying optimal reaction conditions and reactor configurations.

RESEARCH AREA 2

PHOTO-ASSISTED CATALYTIC STEAM GASIFICATION TO SYNGAS FOR DISTRIBUTED POWER GENERATION

PIs: Dr. Xiaoyin Chen and Prof. Johannes Schwank
Students: Tom Westrich and Jordan Martinus

Novel concepts have been pursued to generate syngas using a hybrid process, involving biomass as carbon source and steam generated via solar concentrators. The syngas produced in this way can be directly used for distributed-electricity generation by SOFCs. This process combines photo-catalytic water splitting and catalytic gasification of biomass-derived carbon under solar thermal conditions. It produces syngas at relatively low temperatures; it has a better fuel conversion, less carbon dioxide (CO₂) emissions than coal fueled Integrated Gasification Combined Cycle (IGCC) technology; the process does not require nitrogen oxides (NO_x) and sulfur oxides (SO_x) emissions control equipment.

The objectives of this project are: 1) To gain a detailed understanding of the underlying catalytic mechanisms and develop more effective catalyst formulations; 2) To design an appropriate solar concentrator system to increase solar efficiency; 3) To study the reaction kinetics and optimize the reaction parameters; and 4) To establish the relationship between carbon properties and conversion efficiency.

A promising solution for improving the energy conversion efficiency and reducing CO₂ emission for biomass gasification is the solar thermal gasification where the necessary high-temperature heat is provided using concentrated solar power¹³. High-temperature (≥ 1000 °C) and the novel reactor design derived from heat collection and heat transfer are research issues for solar thermal gasification¹⁴.

We have initiated proof-of-concept experiments, studying the thermal decomposition of model compounds, such as linear or branched hydrocarbons, to directly generate hydrogen and carbon, followed by photocatalytically enhanced steam gasification of the deposited carbon. This concept has been examined for producing hydrogen from water vapor and solid carbon using defined TiO₂-RuO₂ mechanical mixture as a photocatalyst¹⁵. However, this work has not received much attention because of low hydrogen yield and low photocatalysis efficiency.

Many studies have been performed on carbon deposition during steam reforming of methane over nickel, copper, iron, cobalt, platinum, palladium, or ruthenium catalysts⁷. Thermogravimetric methods can be used to quantify carbon deposition rates, by recording the mass increase of coke on a catalyst as a function time¹⁶. Coke can contain

¹³ P.v. Zedtwitz, A. Steinfeld, "The solar thermal gasification of coal-energy conversion efficiency and CO₂ mitigation potential", *Energy* **28** (2003) 441-456.

¹⁴ T. Kodama, "High-Temperature Solar Chemistry For Converting Solar Heat To Chemical Fuels", *Progress In Energy And Combustion Science* **9** (2003) 567-597.

¹⁵ T. Kawai, T. Sakata, "Hydrogen evolution from water using solid carbon and light energy", *Nature* **282** (1979) 283-284.

¹⁶ L.S. Lobo and D.L. Trimm, *Journal of Catalysis*, 1973, **29**, 15-19.

three types of carbon, namely pyrolytic, filamentous, and encapsulating carbon^{17,18,19}, depending on reaction conditions. Pyrolytic carbon stems from homogeneous cracking at high temperatures²⁰. In addition to pyrolytic carbon deposits, tars and other polymers may also coat the reaction vessel at high reaction temperatures (> 600C). On the other hand, filamentous and encapsulating carbons are catalytically formed at lower temperatures. The formation and growth of filamentous carbon follows a rather complex mechanism that is still the subject of intense research. It is believed that decomposition of hydrocarbons on the surface of the nickel particle creates a mass transfer driving force (whether the driving force is a temperature or concentration gradient is still heavily debated) that promotes carbon diffusion through the nickel particles. Once the nickel particle is saturated with carbon, the growth of carbon filaments may take place by forming graphitic layers on the unexposed side of the particle. It is also possible that nickel particles become covered and encapsulated with graphitic sheets, eventually deactivating all catalytic sites.

A series of nickel catalysts were prepared with nickel loadings ranging from 0% to 20%, supported on ceria-zirconia oxide (xxNi/CZO, where xx is the weight percent of loaded Ni). (Table 2). When isooctane was used as model compound, analysis of the coking products showed carbon deposits on 0-5% Ni/CZO were amorphous, rather than graphitic structures. Graphitic signatures were seen at higher nickel loadings (above 15%). This new data is contradictory to the mechanism proposed in the literature, where it is assumed that graphitic carbon planes are crystallized from the carbon-saturated nickel particles^{21,19,22,23,24,25}. Therefore, some mechanistic difference must exist between high and low nickel loading catalysts that would explain this polymorphic discrepancy. Our study also showed a correlation between carbonaceous deposits and nickel particle size (Figure 3).

¹⁷ D. Shekhawat and D. Berry, *Catalysis*, 2006, **19**,184-254.

¹⁸ J.L. Figueiredo, *Materials and Corrosion*, 1998, **49**, 373-377.

¹⁹ J.R. Rostrup-Nielsen, *Catalysis Science and Technology*, 1984, **5**.

²⁰ J.R. Rostrup-Nielsen, *Catalysis Today*, 1993, **18**, 305-324.

²¹ I. Alstrup and M.T. Tavares, *Materials and Corrosion*, 1998, **49**, 367-372.

²² R.T.K. Baker and M.A. Barber, *Journal of Catalysis*, 1972, **26**, 51-62.

²³ J.R. Rostrup-Nielsen and D.L. Trimm, *Journal of Catalysis*, 1977, **48**, 155-165.

²⁴ R.T.K. Baker, *Carbon*, 1989, **27**, No3, 315-323.

²⁵ I. Alstrup, *Journal of Catalysis*, 1988, **109**, 241-251.

Table 2: Physico-chemical properties of NiO/CZO and Ni/CZO

Sample	wt% Ni	NiO/CZO ^a			Ni/CZO ^c			
		BET size ^b (m ² /g)	Average grain		Dispersion size (%)	Ni surface area		Particle size (nm)
			NiO (nm)	CZO (nm)		(m ² /g _{cat})	(m ² /g _{Ni})	
1Ni/CZO	1	57	n.d.	13.4	3.1	0.21	21	33
2Ni/CZO	2	53	n.d.	13.1	3.4	0.45	23	30
5Ni/CZO	5	43	12.6	12.6	2.7	0.90	18	38
					3.2 ^d	1.07	21	32
					2.6 ^e	0.86	17	39
10Ni/CZO	10	42	20.9	12.7	1.6	1.04	10	65
					1.6 ^d	1.08	11	62
15Ni/CZO	15	44	31.1	12.4	1.0	0.99	7	103

^aFresh NiO/CZO after calcining Ni(NO₃)₂/CZO at 600 °C in air.

^bEstimated by Scherrer's equation from XRD patterns.

^cEstimated from CO chemisorption after 600 °C reduction by H₂ flow.

^{d,e}Estimated from H₂ chemisorption after 600 °C and 650 °C calcination, respectively.

Figure 3: Correlation between carbon deposition and nickel catalyst particle size.

Figure 4 is a scanning electron microscopy image of the carbon buildup due to hydrocarbon decomposition. The mechanism of iso-octane decomposition over ceria-zirconia supported nickel catalyst was studied in a modified TA Instruments TGA, with FT-IR used for identification of reaction products. The nickel loading of the catalyst used was 2% (refer to Table 2 for characterization data).

Figure 4: Scanning electron micrograph of carbon deposition on nickel catalyst

The TGA data showed significant carbon deposition (by means of mass gain) within the first 15 minutes of decomposition (Figure 5). This short deactivation time was also seen by Keep and Baker for the decomposition of propane²⁶. However, this timescale is much shorter than is reported in literature for the deactivation of nickel catalysts in POX or SR reactors. In partial oxidation or steam reforming reactors, the deactivating carbon growth usually reacts with either oxygen or steam, respectively. This process continuously regenerates active catalyst sites, allowing for continued reactor operation. The shorter deactivation timescale in our TGA experiments is due to the lack of oxidants in the reactor.

Figure 5: Carbon Deposition Rate (mg C/min/mg Ni) as a function of time (min). Time ($t=0$) is the start of the iso-octane decomposition.

TGA oxidation tests showed little to no carbon deposition at temperatures of 400–450 °C. However, there was a large mass gain at 500 °C and 700 °C. Scanning electron micrographs of decomposition products showed significant carbon filament growth at decomposition temperatures of 500 °C. The 600 °C decomposition led to very few filaments while the 700 °C decomposition had none, although both samples experienced significant mass gain.

In order to develop an understanding of the kinetics of this decomposition reaction, a rate law was proposed based on a simple, single site, three step mechanism.

²⁶ C.W. Keep and R.T.K. Baker, *Journal of Catalysis*, 1977, **47**, 232-238.

It was proposed that iso-octane adsorbed on a surface nickel site, then decomposed into one site-adsorbed carbon and a gaseous heptene molecule. This proposed mechanism is a simplified, preliminary estimate of the actual mechanism. The rate law obtained for the simplified mechanism is as follows:

$$r_{C,formation} = \left(\frac{1}{8}\right)r_{C8,decomposition} = \frac{\left(\frac{1}{8}\right)k_1P_{C8}}{1 + K_2P_{C8} + K_3P_{C7}}$$

To obtain a prediction of the carbon mass deposited over the course of the reaction, this rate was set into a catalytic batch reactor design equation

$$\left(\frac{dN_A}{dt} = -r_A W\right).$$

The solution to this design equation led to an increasing mass of carbon deposited (over time). In order to model the experimental observations, a time-dependant catalyst activity ($a(t) = e^{-\beta t}$) was multiplied by the rate constant, k_1 . In addition, it was assumed that P_{C8} and $P_{C7} \ll 1$, thus, K_2 and K_3 were set to zero. This assumption is based on the FT-IR evidence of reaction products.

There is still one parameter that would be interesting to model: the initial “induction” period. We observed a lag time between the iso-octane introduction point ($t=0$) and the coking period ($t \sim 5$). Literature suggests that this “induction period” is related to the diffusion of carbon through the nickel particles until the particle is saturated with carbon^{21,25}. In order to measure this induction period, a sigmoid function

$$S = \frac{1}{1 + e^{-(t-t_0)}},$$

where t_0 is the induction period, was multiplied into the model’s mass prediction. Under larger t , this function approaches the value of 1, while at small t , this function is approaches 0; thusly, this function should not interfere with the models’ ability to correctly solve for the kinetic parameters (k_1). Given these changes to the model, the prediction of mass gain was very good.

The kinetic parameters of the apparent rate constant, k_1 , were determined from the model comparison to data taken at various temperatures. When this rate constant is plotted on a semi-log plot versus the reciprocal temperature (in K), the apparent pre-exponential factor and activation energies can be extracted. The least-squares best fit line reveals an activation energy of -24 kcal/mol and a pre-exponential factor of 0.029 mm²/s. Other sources in the literature have reported observing a similar negative apparent activation energy barrier (anywhere between -44 and -56 kcal/mol) for the steam reforming of hydrocarbons over nickel^{19,23}.

The 700°C FT-IR spectrum showed significant amounts of thermal decomposition products: isobutene, propene, and methane. Further inspection of the 600 °C decomposition FT-IR spectrum showed similar signs of pyrolysis, but on a much smaller scale. Therefore, coking of nickel catalysts above 600°C could be a result of catalytic as well as pyrolytic decomposition.

As mentioned earlier, the diffusion of carbon through nickel at the beginning of decomposition results in an “induction period” before the mass gain dramatically

increases. Based on the model parameter, t_0 , and knowledge about the transient diffusion through spherical particles, an apparent diffusion coefficient of carbon through nickel (as a function of t_0) of approximately 10^{-14} cm²/s was obtained, which is close to literature values for the bulk diffusion of carbon in nickel ($\sim 10^{-10}$ - 10^{-12} cm²/s)²⁷.

A dedicated reactor system for photo-assisted catalytic steam gasification to syngas has been built (Figure 6). A new quadrupole mass spectrometer with turbomolecular pump and ion pump has been installed and calibrated. The only components still missing are liquid mass flow controllers, that are on back-order and expected to arrive soon.

Figure 6: Reactor system for catalytic steam gasification studies.

²⁷ C.A. Bernardo and L.S. Lobo, *Journal of Catalysis*, 1975, **37**, 267-278

RESEARCH AREA 3

HYBRID EXPERIMENTAL/THEORETICAL APPROACH AIMED AT THE DEVELOPMENT OF CARBON TOLERANT ALLOY CATALYST FOR REFORMING AND SOFC ANODES

PIs: Prof. Suljo Linic and Prof. Johannes Schwank
Student: Eranda Nikolla

The objectives of this project were to

- Utilize quantum Density Functional Theory (DFT) calculations and various state-of-the-art experimental tools, to formulate carbon tolerant hydrocarbon reforming catalysts and SOFC anodes.
- Employ DFT calculations to develop theories on preventing carbon poisoning of the Ni catalysts.
- Test the potential carbon tolerant catalysts in steam reforming of various fuels
- Implement these catalysts as SOFC anodes.
- Utilize various spectroscopic and microscopic tools to characterize the tested catalysts.

The major accomplishments during the reporting period are:

- We have determined, using DFT, that the carbon-tolerance of Ni can be improved by formulated Ni-containing surface alloys that, compared to Ni, preferentially oxidize C atoms rather than form C-C bonds and/or that have lower thermodynamics driving force associated with carbon nucleation on the low-coordinated sites.
- We have found that the formation of a surface alloy leads to the favoring of C oxidation over C-C bond formation and the destabilization of carbon nucleation on the catalyst low-coordinated sites.
- We have tested the stability of various surface alloys, such as Sn/Ni, in steam reforming heavy hydrocarbon fuels.
- We have implemented the Sn/Ni surface alloy as a SOFC anode catalyst.

The development of clean, efficient, and environmentally friendly energy generation systems will require major advances in catalysis. Improved hydrocarbon fuel reforming catalysts and electro-catalysts need to be formulated and synthesized. These catalysts need to perform the desired reactions with utmost efficiencies, at reduced costs, and with improved durability. One of the main issues associated with the catalytic and electro-catalytic reforming of hydrocarbon fuels is that currently used catalysts, such as Ni supported on oxides, deactivate due to the formation of carbon deposits formed in the process of hydrocarbon activation. In this progress report, we describe a hybrid experimental/theoretical effort aimed towards a bottom-up, knowledge-based formulation of carbon-tolerant reforming alloy catalysts that can be used as potential SOFC anode electro-catalysts.

Our objective was to utilize quantum Density Functional Theory (DFT) calculations and various state-of-the-art experimental tools to study the factors that govern the stability of Ni-based reforming catalysts. We demonstrated that monometallic nickel catalysts deactivate due to the high rates of C-C bond formation and the high thermodynamic driving force associated with the nucleation and growth of extended sp²

carbon structures. We have identified Ni surface alloys as potential carbon tolerant catalysts^{28,29,30}. These catalysts could be utilized for catalytic hydrogen production from hydrocarbons and as robust Solid Oxide Fuel Cells (SOFC) anodes for on-cell reforming.

In our approach, we have employed quantum DFT calculations, catalyst synthesis, catalysts testing, and catalysts characterization to identify potential carbon-tolerant alloy catalysts. DFT calculations allow us to obtain, from first principle and with high accuracy, the ground state geometries and energies of relevant reactants, products, and transition states involved in elementary chemical reactions on catalyst surfaces³¹. Reactor experiments and various characterization techniques are applied to test the predictions of DFT calculations. The alloy catalysts were also tested as potential SOFC anodes.

A critical issue with hydrocarbon reforming and on-cell reforming in SOFC cells is that currently used catalysts, such as Ni supported on oxides, facilitate the formation of extended carbon structures which deactivate the catalyst or electro-catalyst (Figure 7a). The formation of carbon deposits can be partially suppressed by an introduction of steam (steam reforming). This approach is not optimal for SOFCs since (i) the presence of steam results in low SOFC energy densities, (ii) significant energy is required to heat the steam to the desired temperature, (iii) the storage of steam requires additional cell compartments making the cell design more complex. It is imperative to design carbon-tolerant reforming (electro)catalysts that can operate with minimal steam concentrations.

Figure 7. (a) Transmission electron micrograph showing a nickel catalyst particle covered by carbon. The carbon deposits were formed during propane steam reforming at 800 °C, using a steam-to-carbon ratio of 1.5. (b) Reaction energies for elementary steps in steam reforming of methane on a Ni(111) surface, obtained by DFT calculations.

²⁸ Nikolla, E. Holowinski, A. Schwank, J. Linic, S., "Controlling Carbon Surface Chemistry by Alloying: Carbon Tolerant Reforming Catalyst", *JACS*, 128 (35), 11354-11355, 2006.

²⁹ Nikolla E., Schwank J., Linic S., "Experimental/Theoretical Approach Aimed at the Development of a Carbon-Tolerant Alloy Catalyst", *Fossil Fuel Cell Program Annual Review*, June 2006

³⁰ Eranda Nikolla, Johannes Schwank, Suljo Linic; "Promotion of the long-term stability of reforming Ni catalysts by surface alloying" *Journal of Catalysis* 250 (2007) 85-93.

³¹ B. Hammer, J.K. Nørskov, "Theory of adsorption and surface reactions" in (eds.) R. Lambert and G. Pacchioni, NATO ASI Series E, Kluwer Academic Publishers, Dordrecht 1997

The elementary-step mechanism for the reforming of hydrocarbons on Ni involves the hydrocarbon activation and fragmentation into H and C adsorbates. The strongly bound carbon atoms or fragments are removed from the Ni surface in C-oxidation reactions yielding adsorbed CO, which further reacts in water-gas shift reaction to form gas-phase CO₂. The oxidizing agents, O and OH, are formed on the catalyst surface in the process of steam activation. In addition to reacting to form CO and CO₂, the C atoms and fragments also react with each other to form extended sp² carbon networks such as graphene sheets or nanotubes. It has been shown that the extended carbon deposits nucleate at low-coordinated sites on Ni³². The formation of extended carbon networks leads to the loss of the catalyst activity. Figure 7b shows the DFT-calculated reaction energies for various elementary steps involved in methane steam reforming on Ni(111). The calculations in Fig 7b support the mechanism discussed above.

Figure 7b also suggests that the life time of a Ni-based catalyst can be prolonged by formulating catalysts that: (i) will preferentially oxidize C atoms rather than from C-C bonds or (ii) will suppress the nucleation and growth of carbon deposits. We have utilized the above discussed molecular mechanistic information to identify Ni-containing surface alloy catalysts that are promising carbon-tolerant alternatives to monometallic Ni. For example, our quantum DFT calculations have shown that small amounts of Sn alloyed into the Ni surface layer enhance the rates of C-oxidation compared to the rate of C-C bond formation. In addition, our DFT studies showed that the nucleation of carbon deposits can also be suppressed with the introduction of Sn. This is illustrated in Figure 8, which shows the calculated adsorption energies – these adsorption energies are a measure of the thermodynamic driving force to form these structures on the catalyst surface – for various carbon nucleation centers on low-coordinated step sites of Ni and Sn/Ni.

Figure 8. DFT calculated adsorption energies for carbon nucleation centers on low-coordination step sites of (a) Ni and (b) Sn/Ni³⁰.

³² H. S. Bengaard, J. K. Nørskov, J. Sehested B. S. Clausen L. P. Nielsen, A. M. Molenbroek, and J. R. Rostrup-Nielsen, "Steam Reforming and Graphite Formation on Ni Catalysts", *Journal of Catalysis*, 2002, 209, 365-384.

Figure 8a shows that the driving force to nucleate the carbon centers on Ni is significantly larger than the driving force on Sn/Ni. For example, the DFT calculated adsorption energies for a C_8 carbon cluster (8 sp² carbon atoms) and a graphene chain on Ni(211) are by 0.23 eV and 0.15 eV per carbon atom respectively more exothermic than for Sn/Ni(211), see Figure 8a. The reason for the Sn-induced change in the thermodynamic driving force to form the carbon nucleation centers is that Sn disrupts the connectivity of the low-coordinated Ni sites.

In addition to above described investigation of the chemistry of carbon structures on Ni and Ni alloys we have also utilized DFT calculations to assess the thermodynamic stability of Sn/Ni surface alloys³⁰.

Figure 9. (a) DFT-calculated formation energies (eV) for various Sn/Ni configurations as a function of Sn surface coordination (number of Sn atoms divided by the total number of surface atoms in the unit cell). (b) Formation energies of Sn/Ni configurations as a function of the Sn chemical potential.

In these studies we have calculated the formation energies of various Sn/Ni structures including: (i) Sn/Ni surface alloys, (ii) Sn/Ni bulk alloys, (iii) Sn adsorbed on Ni substrate, and (iv) separated Sn and Ni. The calculated formation energies are shown in Figure 9b. Figure 9b demonstrates that Sn/Ni surface alloys have the lowest formation energies and that these structures should be stable under typical reforming conditions.

To test the predictions of the DFT calculations we have synthesized and characterized Sn/Ni alloys. Various characterization techniques including STEM, EELS, XPS, and TPR demonstrated that the synthesized material was the Sn/Ni surface alloy³⁰. The performance of the alloy catalysts was examined in a reactor setup in steam reforming of methane, propane, and iso-octane at moderate steam-to-carbon ratios (between 1 and 2). In all experiments, the Sn/Ni catalyst shows no significant deactivation while the Ni catalyst deactivated rapidly. The characterization studies on used catalysts (SEM, TEM, XPS and XRD) showed no signs of carbon formation on Sn/Ni. On the other hand the Ni catalysts were completely poisoned by graphitic carbon deposits.

We have also implemented the Sn/Ni surface alloy catalyst as an anode electro-catalyst for on-cell utilization of hydrocarbons over SOFCs. The anode was composed of a mixture of Sn/Ni catalyst and yttria-stabilized zirconia (YSZ). The electrolyte was made of a thin layer (~ 20 microns) of YSZ and the cathode was composed of a mixture of strontium-doped lanthanum manganite (LSM) and YSZ. Our preliminary results indicate that when isooctane is used as a fuel, the Ni/YSZ/LSM SOFC degrades significantly over time, and the carbon poisoning of the Ni/YSZ anode leads to fuel cell fractures. On the other hand, the Sn/Ni/YSZ/LSM SOFC shows a higher resistance to carbon than the Ni SOFC under identical conditions. One issue worth mentioning is that the formation of carbon deposits as a result of gas-phase combustion reactions before the fuel comes in contact with the anode present a problem for the life span of both the Sn/Ni and Ni electrocatalysts. The formation of these carbon deposits over time puts a significant strain on the seal. The strain results in fuel cell damage. For example, in the case of the Sn/Ni surface alloy anode, the triple phase boundary was free of carbon but the large carbon deposits due to the gas phase reactions resulted in the failure of the seal over time.

In summary, in the work conducted so far, we have utilized DFT quantum calculations to develop molecular insights into the mechanism of carbon poisoning of Ni. We have determined that the long-term stability of reforming electro-catalysts is governed by their capacity (1) to selectively oxidize carbon atoms, while preventing the formation of C-C bonds and (2) to suppress the C nucleation on the low coordinated catalyst sites. DFT studies demonstrated that Sn/Ni favored the C-oxidation reaction over C –C bond formation and hindered the nucleation of carbon at the low coordinated sites. The reactor studies showed that the Sn/Ni catalyst was more stable than monometallic Ni in steam reforming of various hydrocarbons at moderate steam-to-carbon ratios. Sn/Ni alloys also showed promising preliminary results as potential anodes for on-cell utilization of hydrocarbons.

In a quest to minimize the formation of carbon deposits due to gas phase reactions, we have explored various Ni surface alloys for potential use as carbon tolerant reforming catalysts. We showed that Sn/Ni/YSZ catalyst is more carbon tolerant than Ni/YSZ in steam reforming of isooctane at moderate S/C ratios, irrespective of the average size of metal particles and the metal loading. Our DFT calculations have suggested that the reasons for the enhanced carbon-tolerance of Sn/Ni compared to monometallic Ni are: (i) high propensity of Sn/Ni to oxidize carbon and (ii) lower driving force to form carbon deposits on low-coordinated metal sites. We have performed kinetic studies on Ni and Sn/Ni. These studies showed that the overall activation barrier for steam reforming of methane on Ni is by ~ 20 kcal/mol lower than the activation barrier for the same reaction on Sn/Ni. These findings suggest that the enhanced carbon tolerance of Sn/Ni is accompanied by a lower reforming rates on these materials.

The results of this work have been presented in several scientific meetings and received several best paper awards:

- Eranda Nikolla, Johannes Schwank, Suljo Linic, "Experimental/Theoretical Studies Aimed at the Development of Carbon-Tolerant Catalysts", Michigan Catalysis Society Annual Meeting 2006, Dow Chemicals, Midland, MI, May 2006. (Winner of Best Paper Presentation).

- E. Nikolla, “Controlling Carbon Chemistry via alloying: Hybrid Experimental/theoretical Approach”, University of Michigan Engineering Competition 2006, Ann Arbor, MI, March 2006 (Best Poster Award).
- Nikolla E., Schwank J., Linic S., “Hybrid Theoretical/Experimental Approach Aimed at the Development of Carbon Tolerant Alloy Catalysts”, Gordon Research Conference on Catalysis, New Hampshire, Jun 2006 (poster), Best Poster Award (The poster was selected, along with 4 others, among >100 posters presented by Ph.D. students and postdoctoral fellows).
- Linic. S, Nikolla E., “Controlling carbon surface chemistry on Ni by alloying: Carbon tolerant hydrocarbon reforming alloy catalysts”, American Chemical Society National Meeting, Chicago, IL, March 2007.
- Nikolla, E., Schwank J., Linic. S., “Controlling Carbon chemistry by surface alloying”, AIChE Annual Meeting, San Francisco, Ca, Nov 2006 .
- Nikolla E., Schwank J., Linic. S., “Development of carbon tolerant anodes for Solid Oxide Fuel Cells”, North American Catalysis Society Meeting, Huston, TX, May 2007,

RESEARCH AREA 4

POWER ELECTRONICS FOR DISTRIBUTED POWER GENERATION SYSTEMS

PI: Professor Chris Mi

The initial project goal for the power electronics area was to focus on parallel grid connected operations such as stability and grid synchronization. Control strategy and control algorithms for parallel operation of distributed generation system will be developed and validated through experimental work carried out on a scaled down system.

In the previous submitted 6-month progress report, in the power electronics area, we identified two areas that have paramount importance towards a secure and independent energy for the nation.

The “Advanced Thermal Management of Lithium Ion Battery System for Grid Energy Storage Applications” addresses technological issues in thermal management of advanced lithium-ion battery systems for renewable energy system and grid energy storage applications. Lithium-ion battery has the potential to become the most suitable candidate for energy storage in the distributed and renewable energy systems. Thermal management is critical to ensure that lithium-ion batteries provide the desired electrical performance and long life when applied in renewable energy and grid energy storage systems. Lithium-ion battery has the potential of thermal run-away and the operating temperature greatly affects the performance and life cycles of batteries. Advanced battery thermal management systems require accurate prediction of the thermal distribution in battery cells and modules.

The “High Temperature High Power Density Silicon Carbide Converter for Renewable Energy System and Power Grid Applications” will look into technological issues in designing, developing and manufacturing of a new class of converters using silicon-carbide (SiC) power devices. The proposed inverter system is targeted to achieve high power density, high temperature, high efficiency, and high reliability to meet the need in renewable energy system and power grid applications. It will adopt advanced Silicon Carbide power devices, advanced thermal management and cooling systems, advanced packaging methodology, and integrate passive components and gate drive circuits with the inverter system design.

Work accomplished since the 6-month report: Direct-Drive PM Wind Power Generation System with Simplified Power Converter Stages

In the power electronics area, in this phase of the study, we primarily focused on the study of “how distributed and renewable energy systems can be interfaced to the existing power grid, or form a local grid.” Figure 10 shows a typical local grid. In this study the focus is on the AC/DC and DC/AC interfaces between energy sources (such as wind generator, fuel cells, or solar cells) and the grid. In addition, we also designed and tested an isolated DC-DC converter for renewable energy and hybrid vehicle applications. We also developed a scheme for doubly fed wind power generation and its interface with the power grid.

Figure 10. Typical self sufficient farms

Variable speed wind-power generator (VSWG) systems are becoming more and more attractive due to the many advantages of the systems. For example, the annual energy capture of VSWG a system is at least 5% greater than that of a fixed-speed system. The active and reactive power of VSWG systems can be easily controlled. There is no flicker problem to occur with variable-speed turbines. Therefore, there is less mechanical stress for the turbine blades. Rapid power fluctuations are scarce because the high inertia rotor acts as a flywheel. In addition, direct-drive permanent-magnet (PM) wind power generators allow the use of smaller pole pitch than do conventional generators so that higher efficiency can be achieved for the generator. Direct drive system also eliminate the need of gearbox so as to increase the system efficiency.

Direct-drive wind power generators are mostly synchronous machines. Therefore, the frequency and magnitude of the generator output changes with the wind turbine speed. In order to be connected to the utility grid, power converters must be inserted between the generator and the power grid. The most commonly used topology of power converter system for this purpose is shown in Figure 11(a). There are two converters prior to the DC link in the system. One is an AC/DC converter, which converts the variable AC voltage of the generator output to a variable DC voltage. Another is a DC/DC converter that is used to maintain constant DC link voltage. The AC/DC converter is a simple passive rectifier. The DC/DC converter is also unidirectional and can be either a buck or a boost converter depending on the base-speed chosen for the system.

A third power converter, the DC/AC inverter, converts the DC link voltage to AC voltage with frequency and voltage suitable to be connected to the power grid. Because there are two converters prior to the DC link, it is referred to as “two-stage power converter system.” The unidirectional power flow of the converters prior to the DC link

prevents the use of grid power and PM generator to start the wind turbine system. If the wind turbine needs to be started by the PM machine, as required by most direct-drive wind power generation systems, then both the AC/DC converter and the DC/DC converter need to be bidirectional.

In this project, a reduced power converter stage system is proposed as shown in Figure 11(b). In this topology, the former two-stage converters are replaced with one power electronics converter. The DC/DC converter is eliminated. Hence it is a one-stage converter system that can simplify the system and reduce the power converter losses. Besides the simplified structure, this topology can also help start the wind turbine system using the PM generator. At the breezing condition, it is difficult to start the wind turbine because of the existence of detent torque and large inertia of the direct-drive PM generator. The self start feature is a desirable feature for large wind power generator systems. In the one stage converter system, the PWM rectifier will function as a boost converter to keep the DC link voltage constant. The system parameters will affect the adjustable speed range and system efficiency.

In this project, the feasibility and design criteria for the direct-drive PM wind power generator with reduced power converter stages will be discussed. A prototype is designed and simulated to validate the proposed topology. It is shown that the one-stage converter system provide many advantages but impose great challenges to the design of PM generators with regard to the system performance and operating range.

Figure 11. Topologies of direct-drive wind power generation systems. (a). Two-stage converter systems. (b). One-stage power converter systems.

Design and Testing of Silicon Carbide JFET Based Inverter

Silicon carbide (SiC) semiconductor has the characteristics of wide bandgap (3.0eV for 6H-SiC), higher saturation velocity (2×10^7 cm/s), high thermal conductivity (3.3-4.9 W/cmK), low on resistance ($1 \text{ m}\Omega/\text{cm}^2$) and high breakdown electric field strength (2.4MV/cm). Therefore, SiC power devices will have the advantages of larger current carrying capability, higher voltage block capability, high operating temperature, and less static and dynamic losses than traditional silicon (Si) power switches. In

addition, SiC power devices can operate at higher switching frequencies. Therefore, in a inverter system using SiC power devices, the size of its passive components (inductor and capacitor) can be reduced due to the higher frequency operation, so does the associated heatsinks due to lower losses generated as compared with a conventional Si system. At the present time, it is still difficult to produce SiC MOSFET. SiC JFET, on the other hand, is easier to be manufactured and currently is at engineering stage that is being commercialized. As the manufacture technique improves and its mass production can be realized, it is anticipated that there will be more SiC JFET power switches used in power electronic systems.

SiC JFETs are “normally-on” devices. For SiC JFETs to be incorporated in the presently used power converter system designs, there are two possible solutions. One is to use negative voltage to turn it off. For example, a flyback transformer was used to generate the negative gate drive voltage to turn off the SiC JFET. This technique is suitable for DC/DC converters with narrow variation of duty cycle. The other solution is to use a SiC JFET plus a low on-resistance Si MOSFET cascade to form a normally off controlled SiC switch. In this design, the gating circuit same as conventional MOSFETs can be used in the inverter applications like normal MOSFETs. However, the introduction of the additional Si MOSFET will add the system cost and bring additional losses.

In this project, we developed a high-frequency, high-efficiency inverter using SiC JFET modules. In this system, a negative gate drive voltage is used to turn off the SiC JFET, and the gate drive circuit gets power from the DC rail to ensure the safe operation of SiC JFET devices. In addition, the gate driver circuit is optical-isolated and the control logic is the same as traditionally normally off devices. This design enables the integration of the SiC JFET, the driver circuit and the protect circuit into one smart power module. The simulation and experiment results of a SiC JFET inverter and an IGBT inverter demonstrated the low on-state voltage drop and high switching speed prospects of SiC power JFET. The SiC JFET Module inverter using a SiC JFET module shows more than 3% higher efficiency than the new-generation Si IGBT based inverter in wide switching frequency ranges. Figure 12. shows the schematics of the all-SiC inverter. The SiC devices showed significant improvement in switching characteristics. The test results are shown in Figure 13 and Figure 14. The system efficiency of the SiC inverter is higher than that built from conventional Silicon IGBTs, as shown in Figure 15.

Figure 12. The schematics of the all-SiC inverter

(a) SiC JFET with parasitic diode (b) SiC JFET with anti-parallel diode
Figure 13. Reverse recovery current waveforms.

Figure 14. Switching waveforms of Si IGBT. (a) turn-on waveforms. (b) turn-off waveforms.

Figure 15. Inverter efficiency curves of SiC JFET vs. Si IGBT

Papers Presented

1. A paper was presented at the Electric Energy Storage Application and Technology (EESAT) Conference in September 2007 in San Francisco. The paper is entitled "Thermal Modeling and Cooling Design of Li-ion battery for Grid Storage applications."
2. A paper was presented at the IEEE Vehicle Power and Propulsion Conference (VPPC07) in September 2007 in Arlington Texas. The paper is entitled "Coupled Electrothermal Modeling of Li-ion Battery for Hybrid Electric Vehicle Applications."
3. A paper was presented at the 23rd Electric Vehicle Symposium in Los Angeles, California, in December 2007. The paper is entitled "Design and Control of Isolated Bidirectional DC-DC Converter."
4. A paper was submitted to the IET Transactions on Renewable Energy Generation, entitled "Direct-Drive PM Wind Power Generation System with Simplified Power Converter Stages."
5. We developed and tested an all SiC inverter at 300W. And a paper entitled "Experimental Study of Silicon Carbide JFET for Inverter Applications" was submitted to *IEEE Industry Applications Society Annual Meeting*, Calgary, Canada, September 2008.

Recommendations for Future Research

Power electronics is an enabling technology for energy self-sufficient farms, a distributed energy systems proposed by the team. We recommend DOE continue to support our work in the following areas:

1. Development of a low cost, high efficiency power electronic converter system that will integrate a wind unit, fuel cell units that operate from the fuel gas produced in the feedstock-flexible gasifiers in a self-sufficient far, and solar panels, with a battery energy storage system. There are a number of challenges to overcome in developing such systems. To start, the system must be very efficient and capture all the energy possible and store it in the battery or deliver it to a power grid through the power

converter. The power electronic converter must also be intelligent and release the right amount of power when it's needed. The focuses are to develop new topologies that have the potential to provide means to improve system efficiency, while reducing the need for elaborated thermal management systems. These new topologies and related controls must also ensure high reliability and ruggedness.

2. Investigation of SiC power converter technology. SiC semiconductors have been investigated because they offer outstanding power conversion capabilities, include higher operating temperature, higher switching frequency, and lower power. Although a variety of power devices based on SiC technology have been demonstrated, SiC based converters have not been fully investigated. One of the facts is that SiC JFETs are normally "ON" devices; therefore, special gate drive circuits needs to be developed. System-level impacts (technical/economical benefits) of using available SiC devices compared with a silicon based converter needs to be studies through design, modeling, prototyping, characterization and testing. Other issues include the development of advanced gate drive circuits and passive components that will be compatible with the high temperature and high switching frequency operation of SiC devices; and advanced thermal management that can fully utilize the system advantages.
3. Development of a hybrid energy storage. Energy storage is a critical part of distributed energy systems. Ideal energy storage systems shall offer both desired energy density and power density. Lithium-ion batteries can provide high energy densities but the power density is below the expectations for application in renewable and distributed energy applications where a high degree of transient and dynamics require rapid response of energy storage devices. On the other hand, ultracapacitors have very high power density that can handle the fast transients in renewable and distributed energy systems. However, ultracapacitors generally have low energy density. A hybrid energy storage system consisting of a lithium-ion battery and an ultracapacitor offers a compromise of the two. Such system could provide desirable capabilities of high current pulses and extended life of the battery through dynamic load leveling. The proposed work in this area will investigate the modeling and control of such hybrid energy storage system in terms of architecture, efficiency, stability, robustness, power quality, grid compatibility, and system cost effectiveness. The main task is to develop a novel control strategy and associated power electronics circuits for the hybrid energy storage system.

RESEARCH AREA 5

MODELING AND THERMAL MANAGEMENT OF VEHICLE FUEL CELL SYSTEM FOR PROPULSION AND DISTRIBUTED POWER INTO MICRO-GRID

PI: Professor Keshav S. Varde

Student: Pavan Potluri

There has been a great deal of interest in fuel cell (FC) based propulsion system to power light-duty vehicles. The higher efficiency of FC systems compared to the current internal combustion engines, reduction in exhaust emissions and anticipated reduction in greenhouse gases, low noise and concerns over availability of conventional liquid fuels have generated interest in such systems. FC power system, when not used for propulsion, can be used to feed micro-grids or to power residences in case of blackouts or brownouts, and will play an important role as power generators for the energy-self-sufficient farm concept. The premise is that the additional cost of fuel-cell vehicles to consumers can be partially offset by providing grid power support to utilities or major power consumers. The dual use of FC vehicles for clean transportation and grid power support, with some form of shared capital cost or chargeback, could encourage the adoption of these vehicles even at a slightly increased cost to consumers.

Low temperature PEM type fuel cell systems require careful study of reactant flow, reactant states and water and thermal management to optimize their performance³³. At the same time it has to meet the vehicle requirements. Thus, a dual purpose FC system, used for vehicle propulsion and for power generation, requires sizing and energy storage for propulsion, flow and thermal management for vehicular operation and power generation and associated controls for vehicle and grid operations. This requires sizing the FC power system, with associated components, based on vehicle requirements and modeling the system to meet the goals of the project. So far, the sizing of the FC power system has been completed and work is progressing on thermal management of the system.

A dual purpose FC system designed for vehicular propulsion and power generation must have weight, volume, power density, start-up, and transient response similar to the vehicle characteristics with internal combustion engine. Other requirements are: high performance for short time, rapid ramp-up, fuel economy, and ease of access and safety considerations with respect to fuel handling, cost and longevity of durability of the system. The model for the vehicle, powered by a PEM fuel cell system, was developed using PSAT which was modified in this study to incorporate experimentally measured PEM fuel cell characteristics. These characteristics were incorporated in the model in the form of correlations and tables.

A 1 kW PEM fuel cell stack was used in the experimental work. The stack was subjected to steady and transient flow and load variations at different stoichiometric ratios and load and flow parameters. These relationships were then integrated into modified PSAT model for a medium size vehicle. The vehicle parameters for the base vehicle (gasoline powered) are given in Table 3. The simulation was performed for a family type vehicle (medium size vehicle) with specifications given in Table 3 except for

³³ ABI Research, "Hybrid Electric Vehicles – Global Market Assessment, Key Technologies, and Forecasts," 2003.

the weight and performance parameters. The increased weight of the FC with its associated balance of plant and energy storage system contributed to increased weight and differences in vehicle performance parameters.

Table 3. Base Vehicle Data

Approx. vehicle Mass (kg):	1900-2000
Vehicle Frontal Area (m ²):	2.686
Drag Coefficient:	0.417
Rolling Resistance Coefficient:	0.01
Driving Range (km)	500-600

The modified PSAT model was used to achieve compromises between the vehicle weight (including stack and balance of plant components), FC size and vehicle performance parameters. The 1-kW stack characteristics were extended to the vehicle FC power system and were incorporated in the model. The stack was operated in the temperature range of 60-70 °C and 100% reactant humidity; its polarization characteristics are shown in Figure 16.

The vehicle power requirements were estimated in the model based on vehicle acceleration, grade climb, cruising speed, etc. together with the FC characteristics, gaseous hydrogen storage, on-board compressed air supply, etc. It also incorporated various efficiency factors for the compressor, motor, etc.

Figure 16. PEMFC Stack Efficiency (temp ~ 60-70 °C, humidity ~ 100%)

A schematic of the FC and battery energy storage, drive motor, power converters, etc, used in the PSAT model is shown in Figure 17 (from PSAT file). The

traction motor selected for the series FC-battery energy storage system was a UQM PowerPhase-100 brushless permanent magnet motor/generator³⁴ [2].

Fig 17. Series FC and Battery Hybrid Configuration

The motor specifications are given in Table 4. The pre-transmission motor configuration was employed in the system since it provided better blend of vehicle performance characteristics.

Table 4. Traction Motor/Generator Specifications

Torque (Peak)	550 Nm
Motoring Power (Peak)	100 kW
Motoring Power (Continuous)	55 kW
Regen. Power (Peak)	100 kW
Regen. Power (Continuous)	85 kW
Max. Speed (RPM)	5000
Weight	86 kg

The energy storage systems considered in the present model were the batteries (lead acid, NiMH and Li-Ion) or ultra-capacitors. The final selection of the energy storage system was dictated by competitive specific power, specific energy, extended life, ready availability, etc. Despite self-discharge concerns and SOC control complexity, a NiMH battery storage system was selected with the specifications given in Table 5.

Table 5. NiMH Battery Energy Storage System

Voltage	300 V
Nominal Capacity(C/3)	28 Ah
Energy	10 kWh
Number of Cells	300 (50 x 6 cells/module)
Weight	87 kg

³⁴ UQM Technologies Inc.; www.uqm.com

The simulation of the FC vehicle, with its energy storage system, required about 5.8 kg of hydrogen compressed to 35 MPa pressure and stored in light-weight carbon fiber tanks. The vehicle performance parameters for the IC engine powered vehicle (approximate values from matched gasoline powered vehicle) and PEMFC powered vehicle, based on the model, are shown in Table 6.

Table 6. Vehicle Performance Parameters

Category	I.C. Engine Powered	PEM Fuel Cell Powered
Vehicle Mass (kg)	1970	2260
Engine/FC power	Engine: 140 kW	FC: 95 kW
Energy Storage	None	20 kWh Battery System
Maximum Speed	170 km/h	155 km/h
Acceleration 0-100 kph 80-110 kph	8.8 s ~ 5.3 s	11.2 s 6.2 s
Fuel Economy (mpg/kpl gasoline equivalent)	City: 21/8.9 Hwy: 25/10.5	City: 52.3/22 Hwy: 50.2/21.1
Fuel storage (gal/liters or kg)	Gasoline: 16 gal/61 l	Compressed H ₂ : 5.8 kg
Torque coupler	Transmission – 5 speed	Coupler 1.8:1

PEM Fuel Cell for Distributed/Home or Farm Power Generation and Issues

The sizing of the FC system for the vehicle and hydrogen gas storage determined maximum power the system could provide under different charge conditions. A fully charged hydrogen fuel system, with the storage capacity shown in Table 6, would generate about 92 kWh of electrical power at steady conditions. The power generating capability will be lower depending on stored hydrogen energy on-board or available hydrogen energy supply to the FC power generating system. This can be used for local/distributed power generation for emergency use provided appropriate electronics for connecting it to local grid or home supply. The PEM fuel cell system will reject a significant amount of energy in the form of heat. For the system to operate at best operating conditions would require that heat be rejected as it is generated by the PEM fuel cell system.

The heat exchanger in a vehicle is more efficient when the vehicle is moving than when it is at standstill. Thus, a PEM FC powered vehicle, when used for local or distributed power generation would require a heat rejection system to meet power demands.

Next, we will investigate thermal management of the vehicle FC system, with particular attention devoted to heat rejection system when the vehicle is on road and when it is used for distributed power generation. We plan to investigate different heat rejection systems with particular emphasis on size, weight and heat rejection efficiency. The research assistant working on the project is about to complete his studies and we

have a new RA on the project. He will devote his time on the heat rejection system and still continuing on FC bench tests.

FC based power generation offers unique advantages of low to zero emissions, high efficiency and reliability, flexibility in local installation and opportunity for local power generation or distributed power system. FCs are also scalable and can be stacked until the desired power output. Since FCs operate silently, they reduce noise pollution as well as air pollution and the waste heat from a fuel cell could be used for space heating. The idea of localized, distributed power means that electric power can be generated by properly sized fuel cell stack located near to users. Although fuel cell power generation is attractive, the cost of the system has been a detrimental factor. But, fuel cell powered vehicles are gaining momentum because of legislative requirements on fuel economy and emissions. A fuel cell powered vehicle may serve dual purpose: providing propulsion power to the vehicle and power homes or offices when not used as a vehicle. Fuel cell powered vehicles could thus become mobile power stations, as needed and certainly during emergencies or power outage.

This dual-purpose requirement was used to model a PEM fuel cell powertrain for a medium size, family SUV. The size, dimensions and vehicle specifications were selected from one of the current SUVs marketed in the U.S. The fuel cell powertrain, with appropriate energy storage system and controls, was required to meet all the original attributes of the vehicle. Reference [1] gives details of the powertrain and energy storage devices considered in the model.

The performance of the stack was characterized by experimental work on an eight-cell, 252 cm², PEM stack. The stack was operated at controlled thermal parameters at different reactant temperatures and humidity ratios. The stack was subjected to steady state and transient loads with ramping rates of up to a maximum of 800 mA/cm² (and 1 A/cm² for a very short period). The best efficiency of the stack was realized at hydrogen $\lambda = 1.2$, air $\lambda = 2.5$, reactant gas temperatures between 60 and 75 C and relative humidity of 90 to 100%. The stack efficiency was slightly lower at lower temperature and humidity of the reactants.

These characteristics were incorporated in the model in the powertrain simulation model to predict stack size that would yield best fuel economy under urban and highway operations. The maximum power output of the stack, and hence its size, weight, etc, were varied to meet vehicle specifications and requirements. The energy storage systems considered in the analysis were: nickel metal hydride, lithium-ion, and ultra capacitor energy storage.

The results of the simulation show that a PEM fuel cell stack, with a power rating of 40 – 60 kW would be appropriate to meet vehicle specifications and user demands when integrated with an energy storage system. From propulsion considerations, a stack of 50 kW in combination with a Li-Ion storage provided the best efficiency in urban driving, followed by a Ni-MH system [1]. Use of dual energy storage system helped to improve overall stack efficiency because the stack operated at near steady power output over the vehicle duty cycle. A Li-Ion battery storage, in combination with ultra-capacitors, resulted in short acceleration time and improved fuel economy over the urban driving cycle [1].

Whether operated for propulsion or for power generation, a portion of fuel energy supplied to the stack is rejected as heat to the stack coolant. The lower temperature difference between the coolant fluid and ambient air required larger exchanger than in a similar vehicle powered by an internal combustion engine. The larger heat exchanger, with about 75% extra heat transfer surface area, had to be incorporated in the system to account for lower heat transfer rate when the stack was used for power generation from the parked vehicle.

Loading the PEM fuel cell under increasing load (ramped up condition) adversely impacted stack efficiency, as shown in Figure 18, and reduced fuel economy of the vehicle by as much as 3.5 % on urban driving cycle. The power generation capacity of the stack was impacted much because the load was not subjected to transients. Response of the fuel cell to transients in thermal parameters has not been modeled to assess their impact on power generation.

Figure 18. Stack Efficiency Variation During Load Ramping

References

1. Varde, K. S. and Potluri, P.,(2008), PEM Fuel Cell Characterization and its Integration in Simulating a Fuel Cell Powertrain, SAE Paper 2008-01-1796.
2. Varde, K. S. and Potluri, P., Heat Rejection from a Fuel Cell Powertrain Used as Power Generator (in preparation)

RESEARCH AREA 6

CONTROL AND COMMUNICATIONS REQUIREMENTS OF GRID CONNECTED FUEL CELLS

PI: Anna G. Stefanopoulou

Students: Jason B. Siegel

FCs positioned at various locations in the distribution network (12 kV power network) have the ability to function as VAR compensation devices to provide additional voltage stability. FCs have the advantage over photovoltaics (PV) and wind generators (WG) that they can be powered on demand, and that their power output is not a function of environmental conditions. However, reliable FC integration requires deep understanding and quantification of realistic start-up delays^{35,36} and limitations in dynamic FC load following³⁷. This research program addressed the control limits of low-temperature proton exchange membrane fuel cells (PEMFCs) in order to establish a reliable connection to the power grid at the distribution level. The ability to ramp up fuel cell output power to meet the requirements of the load is sensitive to the slowest dynamics in the system. The time constants of the electric power interface are much faster than those of the fuel cell. Therefore, we concentrated on identifying the limiting dynamics of the fuel cell system.

Thermal and liquid water dynamics, drying and flooding in the cell, present the longest time constants³⁸ and have significant impact on overall system efficiency, performance and durability³⁹. Models that accurately capture these water dynamics are needed to optimally control the fuel cell and to develop criteria for controller design. Good models of the system also allow for the design of controllers that use limited sensors combined with a model based observer of the system, thus lowering the cost of hardware implementation. In the case of liquid water dynamics, there are no commercially available sensors to measure the liquid water accumulation within an operating fuel cell, therefore model based observers are critical for evaluating the performance of these systems. The use of cell voltage, which is an inexpensive measurement, as a performance metric is complicated by its parametric nature. The cell voltage is a function of many system variables including; reactant partial pressures, temperature, membrane hydration and the degree of electrode flooding.

³⁵ E. A. Muller, A. G. Stefanopoulou, L. Guzzella, "Optimal Power Control of Hybrid PEM Fuel Cell Systems for an Accelerated System Warm-up," IEEE Transactions Control System Technology, Volume 15, Issue 2, March 2007, Page(s):290 – 305.

³⁶ E. A. Muller, A. G. Stefanopoulou, "Analysis, Modeling, and Validation for the Thermal Dynamics of a Polymer Electrolyte Membrane Fuel Cell Systems," ASME Journal of Fuel Cell Science and Technology, pp. 99-110, Vol. 3, Issue 2.

³⁷ K.-W. Suh, A. G. Stefanopoulou, "Control and Coordination of Air Compressor and Voltage Converter in Load-Following Fuel Cells," International Journal of Energy Research, vol 29, issue 29, pp 1167-1189, Sept, 2005.

³⁸ B.A. McCain, A.G. Stefanopoulou, I.V. Kolmanovsky, "A multi-component spatially-distributed model of two-phase flow for estimation and control of fuel cell water dynamics," Decision and Control, 2007 46th IEEE Conference on, pp 584-589, Dec 2007.

³⁹ *Denise A. McKay, Jason B. Siegel, William T. Ott, Anna G. Stefanopoulou, "Parameterization and prediction of temporal fuel cell voltage behavior during flooding and drying conditions," Journal of Power Sources, Vol 178, Issue 1, pp 207-222, March 2008.

During the reporting period, we developed a high fidelity physics-based fuel cell models that enables detailed analysis of the fuel cell limitations in terms of reactant starvation⁴⁰ and water flooding³⁹. We leveraged our hardware experience with operating fuel cells, to develop testing conditions which can be used for the parameterization of models which predict the water dynamics of PEMFC using cell voltage³⁹. Once the model was parameterized, the next step was to validate the model. Validation of the fuel cell model required measurement of the internal states of the system, such as the accumulation of liquid water inside the cell. Unfortunately there was no way to directly measure liquid water within the cell using our experimental facility.

To address the issue of liquid water measurement we collaborated with the National Institute of Standards and Technology (NIST), and gained access to their Neutron Imaging facility⁴¹. Neutrons are strongly scattered by hydrogen atoms, concentrated in liquid water, and only weakly interact with the other materials used in PEMFCs, such as aluminum and carbon. These images provide a useful tool for in-situ measurement of liquid water content while employing commercial fuel cell materials with realistic cell designs. The use of these materials reduces the possibility of temperature gradients, induced by selection of non-standard materials, which would otherwise greatly impact the formation of liquid water within the cell. An example image is shown in Figure 19, which illustrates the accumulation of liquid water in the anode channel of a 53 cm² PEMFC.

The FC is operated with a dead-ended anode, which greatly reduces the system weight and cost. In this mode of operation hydrogen gas is supplied via pressure regulation and the cell operates with nearly 100% hydrogen utilization. Periodically a solenoid valve has to be opened to purge liquid water from the anode. The increase in air flow through the cathode, referred to as a surge, can also be used to remove any liquid water which has accumulated in the cathode channels. The accumulation of liquid water, and its impact on cell voltage shown in Figure 20 was successfully employed as a diagnostic tool during both anode gas purge and cathode gas surge events under a wide range of temperature, current density, cathode relative humidity, and air stoichiometric conditions.

⁴⁰ *Eric A. Muller, Florian Kolb, Lino Guzzella, Anna G. Stefanopoulou, Denise McKay, "Correlating Nitrogen Accumulation With Temporal Fuel Cell Performance," submitted to the ASME DSCC 2008.

⁴¹ *Jason B. Siegel, Denise A. McKay, and Anna G. Stefanopoulou, "Measurement of Liquid Water Accumulation in a Proton Exchange Membrane Fuel Cell with Dead-ended Anode," submitted to the Sixth International Fuel Cell Science, Engineering and Technology Conference, Denver, Colorado, June 2008.

Figure 19: Neutron images showing the accumulation of liquid water in the fuel cell anode channels.

Figure 20: Liquid water accumulation and voltage degradation

The measurements of liquid water and voltage are well captured by the model for a wide range of operating conditions, approximately 80% of the collected data⁴² as shown in Figure 21. Further development is required in order to expand the range of conditions for which the model can be used.

Figure 21: Comparison of estimated and measured liquid water mass with the model prediction of voltage.

The dynamic limitations associated with nitrogen diffusion and build-up of other inert gas blankets that cover the FC active area and inhibit FC loading were experimentally verified in collaboration with the Swiss Federal Institute of Technology in Zurich, Switzerland. Dynamic drying and flooding phenomena were experimentally validated in our Fuel Cell Control laboratory at the University of Michigan and at NIST using neutron imaging.

Work on combining the models of nitrogen crossover and liquid water dynamics in order to study the resultant impact on cell voltage is already under way through collaboration with ETH, Zurich. Simultaneous measurement of liquid water, using neutron imaging, and nitrogen accumulation, using a gas chromatograph is planned for a

⁴² *Jason B. Siegel, Denise A. McKay, and Anna G. Stefanopoulou, "Modeling and Visualization of Fuel Cell Water Dynamics using Neutron Imaging," American Control Conference, June 2008, Seattle Washington.

second round of testing at NIST in June. Additionally another set of experiments using different gas diffusion mediums and membrane thicknesses will be tested at NIST to verify that our parameterization methodology differentiates the tuned parameters according the actual material variation and cell structure.

The developed FC model is instrumental for increasing the intelligence at the consumer node side of the power grid. Realistic start-up, ramp-up and rump-down predictions of domestic or commercial fuel cells can be utilized at the distribution node-level to schedule resources. The fuel cell model, which includes liquid water dynamics and nitrogen crossover effects, combined with a natural gas fuel processor model^{43,44} will provide a more realistic evaluation of the critical time constants associated with grid-connection and load following ability than models currently used in the literature. Hence our results in modeling, experiments, and diagnostic methods as detailed in the paper (denoted with * in the footnotes of this report section) contribute in a significant way to the understanding of the dynamics and the reliability of the power grid with distributed power generation from FCs.

⁴³ J.T. Pukrushpan, A.G. Stefanopoulou, S. Varigonda, L.M. Pedersen, S. Ghosh, H. Peng, "Control of Natural Gas Catalytic Partial Oxidation for Hydrogen Generation in Fuel Cell Applications," IEEE Transactions on Control Systems Technology, v 13, n 1, January, 2005, p 3-14.

⁴⁴ J. Pukrushpan, A. Stefanopoulou, S. Varigonda, J. Eborn, C. Haugstetter, "Control-Oriented Model of Fuel Processor for Hydrogen Generation in Fuel Cell Applications," IFAC *Control Engineering Practice*, v 14, n 3 SPEC. ISS., March, 2006, p 277-293.

RESEARCH AREA 7

ENERGY STORAGE VIA ADVANCED LITHIUM-ION BATTERY TECHNOLOGY

PI: Johannes Schwank
Student: Liz Ranney

For large energy storage systems, such as the ones envisioned for the energy-self-sufficient farm concept, lithium ion batteries are preferable compared to nickel metal hydride (NiMH) or nickel-cadmium (NiCd) batteries due to their higher energy densities and relatively lower self-discharge rates.

Lithium ion batteries, however, have a too low of capacity and too high of a discharge rate to fully suit the applications for which they serve. This can be explained by describing how current lithium ion batteries work. They consist of a cathode, usually lithium cobalt oxide, and an anode, usually carbon, in a gel-polymer electrolyte. When discharging, lithium ions move from the anode to the cathode and current travels from the cathode to the anode. When charging, lithium ions move from the cathode to the anode while current travels from the charging device to the cathode. The surface area of the cathode limits the amount of lithium ions that the battery can contain. This contributes to the low capacity problem. In addition, the high discharge rate may be explained by the lack of structured pathways in which the lithium ions can travel. The gel-polymer and other lithium ions may interfere with the flow of ions from one electrode to another. Industry also recognizes the need to improve lithium ion batteries. 3M is attempting to increase the capacity of lithium ion batteries by replacing the carbon anode with silicon. One drawback to this solution, however, is that the increased number of lithium ions on the same surface area may cause the batteries to swell resulting in an even shorter lifetime⁴⁵. Sandia National Laboratories is also working to improve lithium ion batteries with the goal of incorporating them into hybrid vehicles as a part of the Department of Energy's FreedomCAR program⁴⁶.

Another solution to the shortcomings of lithium ion batteries could be the placement of nanotubes between the cathode and anode. Nanotubes are desirable due to their high surface area to volume ratio, which would allow for a higher capacity in that more lithium ions could be stored in a small-sized battery. Nanotubes would also provide pathways for ion travel, which would allow the discharge rate to be controlled and slowed. In particular, titania nanotubes could effectively be incorporated into batteries since titanium is a stable, non-corrosive, abundant, and relatively low cost material⁴⁷. If titania nanotubes are successfully implemented in lithium ion batteries to solve the problems of low capacity and high discharge rate, the impact on battery technology would be significant.

⁴⁵ Bullis, Kevin. "3M's Higher-Capacity Lithium-Ion Batteries." *Technology Review*. 25 Oct. 2006. Massachusetts Institute of Technology. 26 Apr. 2007 <<http://www.technologyreview.com/Energy/17653/>>.

⁴⁶ "Sandia Researchers Seek Ways to Make Lithium-Ion Batteries Work Longer, Safer." 16 Jan. 2006. Sandia Corporation. 26 Apr. 2007 <<http://www.sandia.gov/news/resources/releases/2006/renew-energy-batt/battery2.html>>.

⁴⁷ Meng Ni, Michael K.H. Leung, Dennis Y.C. Leung, K. Sumathy, A review and recent developments in photocatalytic water-splitting using TiO₂ for hydrogen production, *Renewable and Sustainable Energy Reviews* (2005), doi:10.1016/j.rser.2005.01.009

Titania nanotubes can be synthesized mainly by the solvothermal method, the hydrothermal method, and anodic oxidation. Lastly, titania nanotubes are prepared by means of anodic oxidation by passing a current through an acidic electrolyte between a cathode, titanium, and an anode, usually a conductor such as copper or platinum. Anodic oxidation has been the focus of our work during the reporting period, since this method allows us to control the dimensions of the nanotubes more effectively, enabling one to tailor the nanotubes to a specific application.

The anode and cathode are thin metal sheets a few centimeters in area immersed in a small volume of electrolyte, which usually contains a small volume of hydrofluoric acid. Voltages applied are generally between 3 Volts and 50 Volts to cause the flow of current. The first step is the formation of an oxide layer on the titanium sheet. This is shown by an exponential drop in current since the oxide layer increases resistance at a constant voltage. Pit formation then begins on the oxide surface. Next, pores form on the surface⁴⁸. This is accompanied by a small increase in current due to the solubility of titania in hydrofluoric acid solutions. A small amount of TiF_6^- is formed, which slightly increases the flow of current while the nanopores form. The last step is nanotube growth. Here, fluoride ions bore the tubes perpendicular to the titanium surface. This is accompanied by a slight decrease in current⁴⁹.

Current research in this area mainly involves finding conditions under which conditions titania nanotubes can be formed and determining their resulting properties. This involves determining the factors that control the nanotube inner diameter, wall thickness, and length. The following paragraphs in this section discuss our assessment of the current work in this field.

The Chen group⁴⁸ used copper as the cathode with an electrolyte containing 0.22-1.1 wt% hydrochloric acid in place of hydrofluoric acid. The experiments took place at room temperature for 30 minutes to two hour durations without stirring. The Chen group's experiments first showed that another acidic compound, such as hydrochloric acid, can be used in place of hydrofluoric acid to form titania nanotubes. They also found that the optimal hydrochloric acid concentration of 0.55 wt. % results in tubes 10 nm in diameter and a few hundred nanometers in length. In addition, they conclude that shorter anodizing times result in more organized tubes while longer anodizing tubes cause the film to dissolve. This conclusion could be misleading because of the anodization time is too short, nanotubes will not be formed at all. Instead, there most likely exists an optimal anodization time for a desired tube length and density. Lastly, they conclude that a porous film, instead of nanotubes, forms at voltages under 10V for their specific electrolyte. Overall, this research is useful in that it proves titania nanotubes can be formed in solutions that do not contain hydrofluoric acid, which is valuable information if the nanotubes are to be formed on large scales.

Prida et al.⁴⁹ also experimented with factors that affect nanotube formation. Titania nanotubes were formed in the 2°C-20°C temperature range using a platinum cathode. The electrolyte was continuously mechanically stirred and contained hydrofluoric acid concentrations of 0.15-0.5% by weight and 1M sulfuric acid.

⁴⁸ Xiaobo Chen, Maria Schriver, Timothy Suen, Samuel S. Mao, Fabrication of 10 nm diameter TiO_2 nanotube arrays by titanium anodization, *Thin Solid Films* (2007), doi:10.1016/j.tsf.2007.03.110

⁴⁹ V.M. Prida, et al., *J. Magn. Magn. Mater.* (2007), doi:10.1016/j.jmmm.2007.02.021

Experiments ran for 20 minutes to 18 hours. The Prida group found that titania nanotubes with an inner pore diameter of 60 nm, wall thickness of about 25 nm, and length of 300 nm could be formed with the electrolyte at lower temperatures. This research proves that titania nanotubes can be formed in fluoride-containing electrolytes, but does not show any correlation between the variables in the experiment and the resulting nanotubes dimensions.

Kaneco et al.⁵⁰ studied the effect of adding methanol to the electrolyte. The titanium and platinum electrodes were separated by 20 mm. The electrolyte was at room temperature and continuously magnetically stirred. In addition, they adjusted the voltage throughout the experiments to maintain a constant current density. The electrolyte contained 1 wt.% hydrofluoric acid and 0, 50, or 90 vol.% methanol. The smallest diameter and highest density of nanotubes were formed in the 50 vol.% methanol electrolyte, with a current density of 10 mA cm⁻².

The Zhao⁵¹ and Xie⁵² groups both used electrolytes containing hydrofluoric acid and phosphoric acid. The Zhao group's electrolyte contained 1 M H₃PO₄ with a hydrofluoric acid concentration of 0.5% by weight. The Xie group, however, used an electrolyte with 0.5 M H₃PO₄ and 0.15 M HF. Both groups also used platinum cathodes and a constant voltage of 20V. The Xie group showed that this setup could achieve nanotubes with average diameters of 260 nm and average lengths of 550 nm.

Macak and Schmuki⁵³ studied the formation of titania nanotubes in viscous electrolytes at varying temperatures. The purpose of their experiments was to determine if viscous electrolytes could reduce inhomogeneities on the titania nanotubes. Platinum was used as the cathode and a constant voltage of 20V was used. The electrolytes used contained either glycerol or ethylene glycol with 0.5 wt.% NH₄F, and the experiments took place at 0, 20, 40, 60, and 80°C. The studies showed that the longest nanotubes were formed in a water-based glycerol electrolyte. These nanotubes had a diameter of approximately 100 nm. They concluded that titania nanotube growth was only possible in the 0 - 40°C range. The results of these experiments show that glycerol is able to control pH fluctuations at the pore tip, and as a result, smooth out inhomogeneities on the nanotubes. The effect of viscous electrolytes is an important finding, and could aid in determining how to incorporate titania nanotubes into battery applications.

Lastly, Mor et al.⁵⁴ studied how the variables in the system affect the shape and growth of titania nanotubes. All of their experiments took place for 45 minutes with a

⁵⁰ Satoshi Kaneco, Yongsheng Chen, Paul Westerhoff, John C. Crittenden, Fabrication of uniform size titanium oxide nanotubes: Impact of current density and solution conditions, *Scripta Materialia* 56 (2007) 373-376.

⁵¹ Jianling Zhao, Xiaohui Wang, Tieyu Sun, Longtu Li, Crystal phase transition and properties of titanium oxide nanotube arrays prepared by anodization, *Journal of Alloys and Compounds* 434-435 (2007) 792-795,

⁵² Yibing Xie, Li Min Zhou, Haitao Huang, Enhanced photoelectrochemical current response of titania nanotube array, *Materials Letters* (2006), doi:10.1016/j.matlet.2006.03.058

⁵³ Jan M. Macak, Patrik Schmuki, Anodic growth of self-organized anodic TiO₂ nanotubes in viscous electrolytes, *Electrochimica Acta* 52 (2006) 1258-1264

⁵⁴ Gopal K. Mor, Oomman K. Varghese, Maggie Paulose, Karthik Shankar, Craig A. Grimes, A review on highly ordered, vertically oriented TiO₂ nanotube arrays: Fabrication, material properties, and solar energy applications, *Solar Energy Materials and Solar Cells* 90 (2006) 2011-2075.

platinum cathode. In addition, the electrolyte contained 0.5 wt. % hydrofluoric acid. Constant voltages of 3, 5, 10, and 20 V were used. The group showed that the addition of acetic acid in a 1:7 acetic acid to electrolyte ratio results in more mechanically robust nanotubes. Also, fluoride concentrations of 0.05 moles/Liter to 0.3 moles/Liter allowed for the formation of nanotubes. They concluded that the nanotube structure is lost when over 23 V are used. In addition, they managed to form conical nanotubes by increasing the voltage from 10 V to 23 V at rates of 0.43-2.6 V/min during the experiment. They also showed that the wall thickness increased with decreasing anodization temperature.

The recent research reported in the open literature tell us how to control the dimensions and properties of nanotubes, and what reaction conditions are conducive to growth of nanotubes, but there are still many unresolved questions, with regard to battery applications of such nanotubes.

Our own experimental approach started by running experiments similar to the ones done by Macak and Schmuki⁵³. We used a copper cathode and titanium anode and explored the effect of a number of different electrolyte compositions. Typical experiments ran for two hours at room temperature. Due to difficulty in forming an oxide layer on the titanium, deionized water was added to the electrolyte to increase conductivity. A new electrolyte was developed, containing 0.5 wt. % NH₄F, 45.7 wt. % water, and 53.8 wt. % glycerol. With this electrolyte, an oxide layer was formed on the sample, and nanotubes were successfully grown.

As first steps toward incorporating nanotubes into a lithium ion battery, we vacuum deposited a proprietary conducting alloy layer that was highly resistant to hydrofluoric acid oxidation on top of a thin polyimide film. A final layer of pure titanium was deposited directly on top of the conductor alloy. Using an anodic process, self-aligned TiO₂ nanotubes were synthesized to precise diameter and length according to the application requirements. The anodic process continued until the Ti at the bottom of the tubes was exhausted upon reaching the HF resistant conducting alloy layer below. The nanotube is now open on one end with a conducting alloy base exposed on the bottom of the tube.

Experiments planned for the future include the development and optimization of several additional steps required to incorporate nanotubes into lithium ion batteries. The applicability of titania nanotubes in these systems creates a need to understand how methods of synthesis affect the nanotube properties and capabilities. Anodic oxidation preparation of titania nanotubes is of particular interest because it creates arrays of ordered, aligned nanotubes perpendicular to a substrate surface. Variation in electrolyte composition, pH, anodization temperature, and electric potential allows for control of the nanotube dimensions. Using the anodic oxidation method, titania nanotubes are prepared by passing a current through an electrolyte between a cathode, titanium, and an anode, usually a conductor such as copper or platinum. Fluoride-containing electrolytes are used most commonly. The first step in the creation of titania nanotubes is the growth of an oxide layer on the titanium sheet according to the following reactions

Since the oxide is less electronically conductive, the formation of an oxide layer can be detected by observing an exponential drop in current since this layer increases the resistance at constant voltage.

The next step is pit formation. Pit formation begins on the oxide surface according to the following reaction:

Next, the pits expand to form pores uniformly spread over the surface. The last step is nanotube growth. Here, the fluoride ions continue to bore into the titania to create the tubes perpendicular to the surface. The rate of nanotube growth is determined by the rate of chemical dissolution of the oxide layer, and nanotube formation is accompanied by a slight decrease in current. The reaction kinetics for oxide layer and nanotube formation are governed by the applied electric current and other components of the electrolyte. The same reactions that cause the growth of pits, pores, and nanotubes cause the formation of the voids between the nanotubes. The voids and tubes must grow in equilibrium for an organized nanotube array to form.⁵⁵

Our synthesis of titania nanotubes started in a clean room environment, where one-inch by three-inch pre-cleaned glass microslides were cleaned with isopropyl alcohol and dried with compressed air. With the microslides inside, the chamber of an SJ-20 E-Beam Evaporator was evacuated to a pressure of approximately 2.0×10^{-6} torr using a cryopump. A 500-nanometer layer of titanium was evaporated onto one surface of the slides. After Ti-deposition, the microslides were cleaned with isopropyl alcohol and dried with compressed air. The titanium was then anodized outside of a clean room environment. During anodization, a 0.2 mm diameter platinum wire (Sigma-Aldrich, 99.9% Pt) was used as a cathode. An microslide area of approximately 3 cm² was immersed in 40 mL of fluoride-containing electrolyte so that the Ti-coated side faced the cathode. The microslide and cathode had a separation distance of 3 cm during experiments. The electrolytes tested contained 0.35, 0.5, and 1.0 wt. % sodium fluoride, and the balance equal amounts of deionized water and glycerol (Sigma-Aldrich, reagent grade 99.9% glycerol) by weight.

The anodizations were performed at room temperature and constant voltage for 15 minutes using a DC power supply (Agilent, E3632A, 0-15V, 7A/0-30V, 4A). The current was monitored using a Data Acquisition/Switch Unit system (Agilent, 34970A) and Agilent BenchLink Data Logger software. During anodization, bubbles formed on the platinum cathode. As the oxide layer, pits, pores, and nanotubes formed, a color shift was observed. The surface of the titanium appeared blue and purple during oxide layer formation. During nanotube formation, the titania surface had bands of pink, green, and yellow. If the anodization time exceeded approximately 20 minutes, dissolution of Ti/TiO₂ was observed. After anodization, the glass microslides were removed from the electrolyte, cleaned with deionized water, and dried under a compressed air stream.

⁵⁵ P. Poizot, S. Laruelle, S. Grugeon, L. Dupont, J.M. Tarascon, Nano-sized transition-metal oxides as negative-electrode materials for lithium-ion batteries, *Nature* 407 (2000) 496.

The microslides were mounted to a metal stage with conducting carbon tape and viewed under a Philips XL30 Field Emission Gun Scanning Electron Microscope. EDS compositional analysis was also performed using the SEM. (Figures 22 and 23).

Due to the superior uniformity of the nanotubes resulting from the 0.5 wt. % sodium fluoride electrolyte at 10 Volts, these samples were chosen for TEM analysis. The titania sides of these microslides were mechanically scraped from the glass onto a copper mesh TEM grid with carbon support film for viewing under 200 kV electrons with a JEOL 2010F Field Emission Gun Analytical Electron Microscope. The AEM was used to obtain TEM and STEM images with the related diffraction patterns in addition to obtain EDS and EELS compositional analyses.

Figure 22. (A) SEM image and (B) EDS spectrum of titania nanotubes made in 0.5 wt. % electrolyte at 10 Volts.

Figure 23. (A) SEM image and (B) EDS spectra of titania nanotubes made in 1.0 wt. % sodium fluoride electrolyte at 15 Volts.

A current density profile consistent with literature was generated for the samples on which nanotubes were formed (Figure 24). This indicates that the sequence of oxide layer formation, pit formation, pore formation, and then nanotube formation was followed in the thin film.

Figure 24. Current density profile resulting from the anodization of a sample 3 cm² in area under the 0.5 wt. % sodium fluoride electrolyte at 10 Volts.

The TEM and STEM images of the titania nanotubes formed in the 0.5 wt. % sodium fluoride electrolyte at 10 Volts verify that the nanotubes have approximately a 50 nanometer diameter, 150 nanometer length, and a 15 nanometer wall thickness. The number density for these samples was approximately 1.44×10^9 nanotubes/mm². A high resolution TEM image indicates that the titania nanotube walls have an amorphous structure. Diffraction patterns taken support that the titania nanotubes are amorphous in structure and that the evaporated Ti substrate layer is polycrystalline.

Figure 25. SEM image, TEM image, and STEM images of titania nanotubes (0.5 wt. % NaF electrolyte) perpendicular to the titanium/glass substrate: (A) viewed under the SEM; (B) at low TEM magnification (40k); (C) using high resolution TEM (600k); (D) bright field STEM; and (E) dark field STEM.

Figure 26. Diffraction patterns showing (A) amorphous structure of TiO_2 nanotubes; and (B) polycrystalline structure of titania substrate.

Compositional analyses were performed using EDS and EELS. The spectra verify that the nanotubes are titania (TiO_2). The spectrum of the Ti substrate layer verifies that no oxide layer is present and that only metallic titanium exists there.

Figure 27. Analysis of the composition showing that the nanotubes are titania and that the substrate remains titanium during the anodic oxidation process where (A) dark field STEM image showing areas surveyed; (B) EDS spectrum at point B; (C) EELS spectrum at point A indicating a composition of nearly 100% titanium, and (D) EELS spectrum at point B indicating the presence of Ti and oxygen in the nanotubes.

Table 7 shows the resulting nanotube diameters and wall thicknesses for the 0.5 wt. % sodium fluoride electrolyte at various electric potentials. The plots in Figure 27 support the trend that tube diameter decreases with increasing electric potential until a voltage, and then it increases. The plots also show the increase in wall thickness with increasing fluoride ion concentration and increasing electric potential.

Table 7: Dimensions of Titania Nanotubes
Made in 0.5 wt. % NaF Electrolyte

Voltage (V)	Average Diameter (nm)	Average Wall Thickness (nm)
8	84	11
10	57	15
12	48	20

CONCLUSION

The research projects carried out under this program have laid the scientific foundation and provided important background technology for the development of compact distributed energy systems that could find applications in concepts such as the energy self-sufficient farm. In addition to the papers provided in the Appendix, other publications based on the research supported are currently in preparation. The relevant manuscripts acknowledging support through this project will be submitted to DOE during the year as they become available.

APPENDIX: PAPERS

Attached are papers presented by:

Professor Chris Mi, who performed research noted in Research Area 4: Power Electronics for Distributed Power Generation Systems

and

Professor Keshav S. Varde, who performed research noted in Research Area 5: Modeling and Thermal Management of Vehicle Fuel Cell System for Propulsion and Distributed Power Into Micro-Grid

Advanced Thermal Design of Lithium-Ion Battery for Grid Energy Storage Applications

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Lithium-ion batteries offer potential advantages in energy density, power density, and cost for use in renewable energy and distributed energy systems. One of the challenges imposed by lithium-ion battery is the thermal management. The best operating temperature of lithium-ion battery is from -10°C to 50°C . An effective thermal management system is critical to maintain the health and life span of the battery. A good thermal management system starts with accurate prediction of the thermal conditions of the battery. This paper is aimed to design an effective thermal management system for the lithium-ion battery pack, including estimating the thermal loss of the battery pack based on electric characteristics and experiments; predicting the temperature rise of the battery pack based on the test results of a single cell, and modeling the temperature gradients of the battery pack under different operating conditions.

This paper presents the study on the thermal modeling of a lithium-battery pack. The pack consists of 48 lithium-ion battery cells. All the 48 cells are electrically connected in series to provide needed voltage. The mechanical arrangement of the 48 cells is shown in Fig. 1 (a), where the pack is divided into two groups. Each group has 24 battery cells stacked together with aluminum cooling fins in between the cells. Fig. 1 (b) further shows the cross section of each battery group. The battery pack is fitted into a metallic case, with thermal insulation inserted between the battery and the case. The cooling fins run through the battery and extends beyond the battery at the bottom to form a cooling channel to allow cooling to flow. Therefore, it can be assumed that there is no heat exchange between the ambient and the battery. Battery heat is carried out by the cooling fins. The cooling air takes away heat from the cooling fins.

Fig. 1. Arrangement of the lithium-ion battery pack. (a). Battery without the casing. (b). Cross section of the battery pack. The cooling fins run between battery cells and extend beyond the battery. The battery pack is fitted into a metallic case, with thermal insulation inserted between the battery and the case.

In order to determine the heat generation in the battery packs during operation, we performed test on a single cell during rated-current charge and discharge. The battery cell under test was placed in an ambient without external heating or forced air disturbance. The temperature rise of the cell during cell charge and discharge is shown in Fig. 2. The flat temperature profile, after a long period of operation, indicates that a steady state is reached. Examination of the thermal history shows that the temperature difference is $32.92^{\circ}\text{C} - 25.22^{\circ}\text{C} = 7.70^{\circ}\text{C}$, when steady state is reached. This averaged temperature is calculated using the average of temperature

readings over one cycle. Since the test cell is exposed in the air without any forced air cooling, there only exists radiation and nature convection. The estimated heat in the cell was 2.7W. The heat generation can also be calculated using the battery impedance and charge rate. The measured cell impedance is 3.263mΩ. The calculated loss of the battery cell is 4.08W during discharge and 1.02W loss during charge. The average loss is $(4.08 * 156 \text{ seconds} + 1.02 * 312 \text{ seconds}) / (156s + 312s + 5s + 5s) = 2.0 \text{ W}$. This is lower than the estimated heat of 2.71W. The difference could be introduced by the calculation error and inaccuracy of the internal impedance. Besides, this loss may not include the conduction loss in the electrodes.

The 48-cell battery pack is analyzed using both analytical and numerical method. The temperature of the battery during normal charge/discharge is shown in Fig. 3. The numerical and analytical results are compared in Table I. It can be seen that the results from the two methods are consistent.

Fig. 2. Temperature rise of a single battery cell as a function of time during constant charge/discharge.

Fig. 3. Battery temperature rise. X-axis: length direction of the battery; y-axis: height of battery (in cm).

We also studied the effect of fin length. Table II shows the temperature rise for fin length of 5mm, 10mm, 15mm and 25 mm. It can be seen that for the given conditions, only 25mm will be able to satisfy the operating requirement.

Table I Comparison of Temperature Rise Calculated Using Analytical and Numerical Methods

	Numerical	Analytical	Difference
Lowest Temperature rise (°C)	11.0	10.8	1.8%
Maximum Temperature rise (°C)	16.4	17.3	9.5%
Temperature gradient (°C)	5.4	6.5	1.1°C
Inlet/outlet air temperature difference (°C)	16.3	15.8	3.2%
Highest pack temperature (°C)*	40.7	39.6	2.8%

Table I Temperature Rise with Different Fin Size

Fin height	5mm	10mm	15mm	25mm
Maximum temperature rise (°C)	43.32	34.23	30.08	23.74
Lowest temperature rise (°C)	33.52	21.97	16.70	10.81
Average Temperature rise (°C)	38.42	28.10	23.39	17.28

Conclusions

This paper presented the thermal analysis and design of lithium-ion battery for potential PHEV applications. The analytical calculations and numerical simulations show that in order to effectively cool the battery pack, a minimum 25mm cooling fin is needed. Transient analysis shows that it takes long time to cool battery to below acceptable operating temperature under extreme initial temperature. The prototype is being developed and further experiments will be carried out to validate the design.

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Advanced Electro-Thermal Modeling of Lithium-Ion Battery System for Hybrid Electric Vehicle Applications

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Abstract — The successful implementation and commercialization of hybrid electric vehicles (HEV) rely largely on energy storage systems. Lithium-ion batteries offer potential advantages in energy density, power density, and cost for this purpose. One of the challenges imposed by lithium-ion battery is the thermal management. The best operating temperature of lithium-ion battery is from -10°C to 50°C . An effective thermal management system is critical to maintain the health and life span of the battery. A good thermal management system starts with accurate prediction of the thermal conditions of the battery. This paper is aimed to evaluate the thermal management system of a lithium-ion battery pack designed for HEV applications, including estimating the thermal loss of the battery pack based on electric characteristics and experiments; predicting the temperature rise of the battery pack based on the test results of a single cell, and modeling the temperature gradients of the battery pack under different operating conditions.

Index Terms — Battery, HEV, hybrid electric vehicle, lithium-ion, plug-in hybrid electric vehicles, thermal management.

I. INTRODUCTION

LITHIUM-ION batteries are considered the only viable energy storage device for hybrid electric vehicle (HEV) applications [1-3]. Although lithium-ion battery has been widely used in electronics devices, it is not yet ready for use in HEV due to the thermal limitations [4-9]. There have been studies on lithium-ion battery thermal issues [10], mostly focused on the electro-chemistries. This paper presents the study on the thermal modeling of a lithium-battery pack suitable for a HEV application. The vehicle will contain one or more battery backs with each pack consists of 48 lithium-ion battery cells. All the 48 cells are electrically connected in series to provide needed voltage. The mechanical arrangement of the 48 cells is shown in Fig. 1, where the pack is divided into two groups. Each group has 24 battery cells stacked together with aluminum cooling fins in between the cells.

Fig. 1. Arrangement of the lithium-ion battery pack without the casing. The battery pack contains 48 cells with 24 cells in each of the two groups. The 48 cells are electrically connected in series.

Fig. 2. Cross section of the battery pack. The cooling fins run between battery cells and extend beyond the battery. The battery pack is fitted into a metallic case, with thermal insulation inserted between the battery and the case.

Fig. 2 further shows the cross section of each battery group. The battery pack is fitted into a metallic case, with thermal insulation inserted between the battery and the case. The cooling fins run through the battery and extends beyond the battery at the bottom to form a cooling channel to allow cooling to flow. Therefore, it can be assumed that there is no heat exchange between the ambient and the battery. Battery heat is carried out by the cooling fins. The cooling air takes away heat from the cooling fins.

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II. ESTIMATION OF THE HEAT GENERATION IN A SINGLE BATTERY CELL

In order to determine the heat generation in the battery packs during operation, we performed test on a single cell during rated-current charge and discharge. The battery cell under test was placed in an ambient without external heating or forced air disturbance. The temperature rise of the cell during cell charge and discharge is show in Fig.3. The flat temperature profile, after a long period of operation, indicates that a steady state is reached. Examination of the thermal history shows that the temperature difference is $32.92 - 25.22 = 7.70^\circ\text{C}$, when steady state is reached. This averaged temperature is calculated using the average of temperature readings over one cycle. Since the test cell is exposed in the air without any forced air cooling, there only exists radiation and nature convection.

For the thermal system under consideration, the Rayleigh number can be calculated as a function of characteristic length L ,

$$Ra_L = \frac{g\beta(T_{\text{battery}} - T_{\text{air}})L^3}{\alpha\nu} \quad (1)$$

where g is natural gravity, β is the thermal expansion coefficient: $\beta = 0.00333$ (1/K), T_{battery} and T_{air} are the battery and air temperature respectively, and other parameters are listed in Table I.

For a battery arranged vertically, the Rayleigh number $Ra_L = 1.16 \times 10^6$ and the Nussel number and the heat transfer coefficient for the vertical surface are determined by the following expressions:

$$\overline{Nu}_L = \left(0.825 + \frac{0.387(Ra_L)^{1/6}}{(1 + (0.492 / Pr)^{9/16})^{8/27}} \right)^2 = 17.2 \quad (2)$$

$$h_v = \frac{\overline{Nu}_L \times k}{L} = \frac{17.2 \times 0.0263}{0.118} = 3.84 \text{ (W / (m}^2\text{K))} \quad (3)$$

For the top horizontal surface, $Ra_L = 9.71$, $Nu_L = 0.54Ra_L^{1/4} = 0.95$, and

$$h_t = \frac{Nu_L \cdot k}{L} = 10.45 \text{ (W / (m}^2\text{K))}.$$

For the bottom horizontal face, $Nu_L = 0.27$, $Ra_L^{1/4} = 0.477$,

$$h_b = \frac{Nu_L \cdot k}{L} = 5.23 \text{ (W / (m}^2\text{K))}.$$

The heat transfer rate due to radiation, assuming that the surface of the battery is painted black and the emissivity is 1.0, is calculated as,

Fig. 3. Temperature rise of a single battery cell as a function of time during constant charge/discharge.

TABLE I
AIR PROPERTIES AT TEMPERATURE 300K

Temperature	Density (ρ)	Kinematic Visc (ν)	Thermal Conductivity (k)	Thermal Diff (α)	Prandtl No. (Pr)
	kg/m ³	m ² /s	W/m-K	m ² /s	
300	1.1614	15.89e6	0.0263	22.5e6	0.707

$$h_{\text{rad}} = \varepsilon\sigma(T_{\text{battery}}^2 + T_{\text{air}}^2)(T_{\text{battery}} + T_{\text{air}}) = 6.23 \text{ (W / (m}^2\text{K))} \quad (4)$$

Total heat removed by air from the surface of the battery is the same as the heat generated by the battery. Thus the total heat generated by the battery cell is

$$\begin{aligned} Q_{\text{gen}} &= A_{\text{total}} h_{\text{rad}} (T_{\text{battery}} - T_{\text{air}}) + 2A_v h_v (T_{\text{battery}} - T_{\text{air}}) \\ &\quad + A_h (h_t + h_b) (T_{\text{battery}} - T_{\text{air}}) \\ &= 2.71 \text{ W} \end{aligned} \quad (5)$$

The heat generation can also be calculated using the battery impedance and charge rate. The measured cell impedance is 3.263m Ω . The calculated loss of the battery cell is 4.08W during discharge and 1.02W loss during charge. The average loss is $(4.08 * 156 \text{ seconds} + 1.02 * 312 \text{ seconds}) / (156\text{s} + 312\text{s} + 5\text{s} + 5\text{s}) = 2.0 \text{ W}$. This is lower than the estimated heat of 2.71W. The difference could be introduced by the calculation error and inaccuracy of the internal impedance. Besides, this loss may not include the conduction loss in the electrodes.

III. NUMERICAL ANALYSIS

A. Single Cell

In 2D static FEA model, the loss is assumed to be evenly distributed over the whole battery cell including packaging material with a total loss of 2.71W. Assume that there is nature convection from the four sides of the battery cell, ambient temperature is 25°C, and use the nature convection coefficient derived from the last section. The average

Fig. 4. A single battery cell temperature rise calculated using 2D FEA static analysis. The air temperature is 25°C.

Fig. 5. Battery module temperature rise calculated using 2D FEA static analysis. The module consists of four cells vertically compressed together with polymer packaging, without cooling fins. The air temperature is 50°C.

temperature-rise is 7.5°C; maximum temperature-rise is 8.6°C; and the gradient is 2.3°C among the battery. Both the temperature rise and the gradient result are slightly lower than the testing results with the error being less than 3%. The cell temperature distribution is shown in Fig. 4.

B. Four- Cell Module

In order to validate the calculation of heat generation and temperature-rise, we performed a comparison of estimated temperature against the test results on a four-cell battery module. The analytical and numerical methods are consistent with the test results. The temperature gradient of the module is shown in Fig. 5. It shows that with four cells packed together without cooling, the temperature-rise is 100% higher than the single cell.

IV. DESIGN ANALYSIS OF THE 48-CELL BATTERY PACK

The 48-cell battery pack is analyzed using both analytical and numerical methods. The 48 cells are divided into two groups with each group consists of 24 cells. Since the two groups of batteries are packed in the same length direction as shown in Fig. 1, the cooling air pass through the first group to reach the second group. The average temperature rise and

TABLE II
TEMPERATURE RISE WITH DIFFERENT FIN SIZE

Fin height	5mm	10mm	15mm	25mm
Maximum temperature rise (°C)	43.32	34.23	30.08	23.74
Lowest temperature rise (°C)	33.52	21.97	16.70	10.81
Average Temperature rise (°C)	38.42	28.10	23.39	17.28

Fig. 6. Battery temperature rise. X-axis: length direction of the battery; y-axis: height of battery (in cm). Lower left corner has inlet air temperature at 9°C, top right corner has temperature of 40°C.

TABLE III
COMPARISON OF TEMPERATURE RISE CALCULATED USING ANALYTICAL AND NUMERICAL METHODS

	Numerical	Analytical	Difference
Lowest Temperature rise (°C)	11.0	10.8	1.8%
Maximum Temperature rise (°C)	16.4	17.3	9.5%
Temperature gradient (°C)	5.4	6.5	1.1°C
Inlet/outlet air temperature difference (°C)	16.3	15.8	3.2%
Lowest pack temperature (°C)*	9.0	9.0	-
Highest pack temperature (°C)*	40.7	39.6	2.8%

*Note: Inlet temperature is 9°C

maximum temperature rise for different fin heights are shown in Table II, calculated by analytical method. It can be seen that, in order to maintain the battery within the desired 40°C, a minimum 15mm fin length, and cooling air below 10°C is required. Fig. 6 shows the temperature distribution inside the battery pack.

V. TRANSIENT PERFORMANCE OF THE BATTERY PACK

One scenario for HEV battery is the extreme heat generated by the sun inside the vehicle compartment when the vehicle is parked under the sun in the summer time. It is estimated that the vehicle compartment temperature can get to 55°C or above. This part of study is to find out how long it takes to cool the battery to below the threshold temperature of 40°C when the battery can be activated.

Analytically, the battery temperature satisfies the following equation:

$$T - T_{air} - \frac{Q}{Ah} = \left(T_i - T_{air} - \frac{Q}{Ah} \right) \exp \left(-\frac{Ah}{mC_v} t \right) \quad (6)$$

$$t = \left(\frac{mC_v}{Ah} \right) \ln \left(\frac{T_i - T_{air} - Q/Ah}{T - T_{air} - Q/Ah} \right) = \left(\frac{mC_v}{Ah} \right) \ln \left(\frac{T_i - T_{air}}{T - T_{air}} \right) \quad (7)$$

where $mC_v = m_b C_b + m_{AL} C_{AL}$: subscript b stands for battery and AL for aluminum sink, Q is the heat generation of the battery, A is the area exposed to the air flow, t is the time, T is the battery temperature, T_i is the initial temperature, T_{final} is the final temperature of the battery, and A_h is the cooling surface area and h is the heat transfer coefficient.

Consider the cooling of the 48-cell battery pack initially heated up to 55°C. For this case, $Q = 0$ and $T_i - T_{air} = 45^\circ\text{C}$, assuming that the cooling air is at 10°C. Since there is a 15°C temperature difference between inlet air and outlet air, the final battery average temperature needs to be within 30°C in order to maintain the maximum temperature within 40°C. The time can be calculated as follows,

$$m_{Al} = \rho_{Al} V_{Al} = 1.68 \text{ kg} \quad m_b = \rho_b V_b = 5.9 \text{ kg} \quad (8)$$

$$mC_v = m_b C_{v,b} + m_{Al} C_{v,Al} = 26075.21 \text{ J / K} \quad (9)$$

$$Ah = 21.69 \text{ W / K} \quad (10)$$

$$\ln \frac{T_i - T_{air}}{T_{final} - T_{air}} = \ln \frac{45}{20} = 0.811 \quad (11)$$

$$t = \left(\frac{mC_v}{Ah} \right) \ln \left(\frac{T_i - T_{air}}{T - T_{air}} \right) = 979 \text{ sec} \quad (12)$$

Therefore, it needs 16 minutes before the battery can be activated to drive the vehicle.

In order to validate the analytical results, FEA is used to calculate the transient temperature of the battery under extreme initial temperature conditions. A simple FEA model was build containing only one cooling fin and two-half batteries on each side of the cooling fin using symmetrical conditions as shown in Fig. 7. It is assumed that there is no heat exchange between battery cells, and all surfaces are thermally insulated except the bottom of cells. It means that battery temperature across the width direction is the same; and temperature rises across the height direction. Across the length (channel) direction, air temperature rises as it pass through the cooling channels. This can be seen as shown in Fig. 6.

The transient temperature is shown in Fig. 8. It can be seen that it takes 902 seconds to cool the battery from 55°C to below average 30°C. This is consistent with the analytical method with error being less than 8%.

Fig. 7. Battery model used for the transient calculations in FEA.

Fig. 8. Battery temperature under extreme initial temperature of 55°C.

VI. CONCLUSION

This paper presented the thermal analysis and design evaluation of lithium-ion battery for potential HEV applications. The analytical calculations and numerical simulations show that in order to effectively cool the battery pack, a minimum 25mm cooling fin is needed. The prototype is being developed and further experiments will be carried out to validate the design.

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Isolated DC-DC Converter for Hybrid Electric Vehicle Energy Management Applications

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Abstract

Hybrid electric vehicles (HEVs) offer many advantages, such as high fuel economy, low emissions, and possible silent operation. In the current HEV designs, there are usually two or more different DC voltage systems for different purposes of the vehicle operations. Galvanic isolation is often needed for safety concerns, especially in military vehicles. Bidirectional DC-DC converters are therefore used to interconnect different DC voltage bus and transfer energy between two different DC voltage buses. For example, in one of the developed military HEV systems, one DC-DC converter converts the high voltage (200-300V) from HEV powertrain battery to low voltage (~14V) for auxiliary needs in the vehicle, while the other converts 300V powertrain battery voltage to 600V to supply the powertrain motors. High efficiency, compact size, lightweight, and reliability are all essential requirements for DC-DC converters for and HEVs.

This paper details the development of an isolated bidirectional DC-DC converter for HEV energy management use, with focuses on the steady state operation analysis. A phase-shift controlled dual bridge topology is developed to achieve the requirements. The continuous and discontinuous operation modes are analyzed and the boundary for continuous operation was studied. The voltage ripple of the output was also derived. The proposed converter was simulated and a 10kW prototype is built and tested. The experimental results of the converter's steady state operation and transient operation validated the design and simulation.

Keywords: Hybrid electric vehicle, average model, DC-DC converter, bi-directional converter, isolation, two time scale

1. Introduction

In hybrid electric vehicles (HEVs), difference voltage systems exist as shown in Fig.1. In order to take full advantage of the powertrain motor and associated power electronics devices, high voltage is employed to reduce the complexity of electric drive system and improve efficiency [1-3, 7]. Current HEVs typically [3] employs a 600V to 800V DC bus voltage for driving motor and 200V to 300V for hybrid battery or ultra capacitor. Therefore, there is a need of a high power bidirectional converter to transfer power between the two voltage systems. The bidirectional DC-DC converter is a key component in HEVs to provide buck, boost, and bidirectional power flow. The converter provides flexibility for the rest of the power electronics circuit in the hybrid powertrain, so that high efficiency, high power density, lower devices stress and high reliability can be achieved [4]. At the mean time there are other auxiliary components which operate at 14V or 42V. Auxiliary equipment, such as air-conditioner, consumes power from the auxiliary battery. In HEVs, the engine may be turned off to save fuel. The auxiliary battery could be discharged quickly while the engine is turned off. Therefore, there is a need of a low power bidirectional DC-DC converter to transfer power between the hybrid battery and the auxiliary battery.

In military vehicles, the hybrid battery is used to replace the stationary portable power generators to supply power to command centers and other needs. Isolation is needed in military vehicles to provide safe operation for the equipment that is operated on the hybrid battery.

Fig. 1. The electrical systems in a series HEV

2. Circuit Configuration

Fig. 2 shows the schematic of the isolated bidirectional DC-DC converter designed for an HEV, which consists of dual H-bridges and a high frequency transformer. The high frequency transformer provides the required isolation for safety and voltage matching between low voltage bus and higher voltage bus. The transformer's leakage inductor serves as the instantaneous energy storage. The first H-bridge provides a square wave AC voltage to the primary winding of the high frequency transformer. The bridge consist of four switches Q_1 , Q_2 , Q_3 and Q_4 , which are IGBTs power devices for high power applications [6]. The second H-bridge, also consisting of four switches Q_5 , Q_6 , Q_7 and Q_8 , are connected directly to secondary winding of the transformer. The second bridge and the leakage inductance of the secondary winding of the isolation transformer form a boost converter. The boost operation at the second H-bridge is fulfilled by phase shift control between the first and secondary side of the transformer. The operation is bidirectional, e.g., each H-bridge can be considered as primary or secondary depending on the direction of power flow.

Fig. 2. Isolated dual bridge bidirectional converter for HEVs

3. Steady State Operation

The first H-bridge converts the DC voltage to a square wave AC voltage. The second H-bridge operates in the boost mode. The turns-ratio of the transformer is n , the transformer primary voltage is V_1 , the transformer second voltage is nV_1 ; DT_s is the phase shift between the two bridges, where D is the duty cycle in a half period T_s ; I_{Ls} is the current of the leakage inductor, and V_2 is the output voltage. In this analytical analysis, we also neglected: (a) dead time; and (b) switch dynamics.

There are two difference operation modes based on the output current with a boundary between the two operation modes. The boundary conditions are very similar to the non-isolated bust converter, where the

inductor current increases from zero in steady state at the beginning of the switching cycle, and drops to zero at the end of the switching cycle. But there is no discontinuous mode, e.g. the inductor current will not be zero in both above and below the boundary conditions. In this paper, for the ease of terminology, we will still name these operation modes continuous mode and discontinuous mode. In “discontinuous” mode, the inductor current is in fact still continuous. Here we may refer to that the free-wheeling current in the diode will become zero (discontinuous). The typical waveform over one cycle operation is shown in Fig. 3.

3.1 Continuous Operation

During the continuous operation mode of the phase shift operation, the inductor current increases from a negative value at the beginning of the switching cycle in steady state. There are four states in each switching cycle, as shown in Fig. 3 (a).

Segment 0: $[t_0, t_1]$. In this Segment, Q_6 and Q_7 are turned on. The current in inductor L_{sl} increases linearly, from a negative value. The total current ripple during this time interval is

$$\Delta I_{L_{sl}} = \frac{DT_s}{L_{sl}} V_{L_{sl}} \quad (1)$$

Or

$$\Delta I_{L_{sl}} = \frac{DT_s}{L_{sl}} (V_2 + nV_1) \quad (2)$$

Segment 1 $[t_1, t_3]$. In this Segment, switch Q_6 and Q_7 are turned off and switch Q_5 and Q_8 are turned on. Although Q_5 and Q_8 are turned on, there is no current flow through these switches. Diodes D_6 and D_7 freewheel.

The leakage inductor current ripple during this time interval is

$$\Delta I_{L_{sl}} = \frac{(1-D)T_s}{L_{sl}} (V_2 - nV_1) \quad (3)$$

At the end of the switching cycle, inductor current is not zero.

Segment 3 $[t_3, t_4]$. The transformer primary voltage is reversed, so nV_1 changes direction. Since the inductor current is not zero, Diodes D_6 and D_7 continue to freewheel until the inductor current reaches zero, when Q_5 and Q_8 starts to conduct. The current ripple in L_{sl} is

$$\Delta I_{L_{sl}} = \frac{DT_s}{L_{sl}} (nV_1 + V_2) \quad (4)$$

Segment 4 $[t_4, t_5]$. Q_5 and Q_8 are turned off, and D_6 and D_7 begin to freewheel. The current ripple in L_{sl} is

$$\Delta I_{L_{sl}} = \frac{(1-D)T_s}{L_{sl}} (V_2 - nV_1) \quad (5)$$

From the symmetry of the inductance current, $i(t_0) = -i(t_3)$ in Fig. 4. From (1) ~ (4), the initial inductor current can be obtained as $i(t_0) = \frac{1}{4f_s L_s} [(1-2D)V_2 - nV_1]$ and the maximum current can be obtained

as $I_{\max} = \frac{1}{4f_s L_s} [-(1-2D)nV_1 + V_2]$. The average current in inductor is

$$\bar{I} = \frac{1}{2T_s} [(i_{\max} + i(t_0))DT_s + (i_{\max} - i(t_0))(1-D)T_s] = \frac{1}{2f_s L_s} D(1-D)V_2 \quad (6)$$

The supplied power is equal to the output power neglecting transformer and the switch losses

$$P_1 = nV_1 \bar{I} = \frac{nV_1 V_2}{2f_s L_s} D(1-D) = P_o = \frac{V_2^2}{R_L} \quad (7)$$

Therefore

$$V_2 = \frac{nV_1}{2f_s L_s} R_L D(1-D) \quad (8)$$

The waveforms of the continuous operation are illustrated in Fig. 3(a).

Fig. 3. The typical voltage and current waveforms

3.2 Boundary Conditions

At boundary conditions, as shown in Fig. 3(b), the inductor current reaches zero at the end of the switching cycle. The operation States are the same as in continuous mode.

Because $t_6 - t_4 = (1-D)T_s$, the total current ripple in L_{sl} is

$$I_o = \frac{1}{2} \Delta I_{L_{sl}} = \frac{DT_s}{2L_{sl}} (V_2 + nV_1) = \frac{(1-D)T_s}{2L_{sl}} (V_2 - nV_1)$$

&

$$V_2 = \frac{nV_1}{1-2D} \quad (9)$$

3.3. “Discontinuous Mode”

With further output current decrease, the operation enters a mode similar to the discontinuous mode in boost converters. In this mode, the inductor current reaches zero before the end of the switching cycle, as shown in Fig. 3(c). There are six operation segments in this mode.

Segment 0: $[t_0, t_1]$. In this Segment, Q_6 and Q_7 are turned on. The current in inductor L_{sl} increases linearly from a positive value I_1 to $I_{\max}$. The current ripple during this time interval is

$$\Delta I_{L_{sl},1} = I_{\max} - I_1 = \frac{DT_s}{L_{sl}}(V_2 + nV_1) \quad (10)$$

Segment 1 $[t_1, t_2]$. In this Segment, switch Q_6 and Q_7 are turned off and switch Q_5 and Q_8 are turned on. Although Q_5 and Q_8 are turned on, there is no current flow through these switches. Diodes D_6 and D_7 freewheel. The leakage inductor current ripple during this time interval is

$$\Delta I_{L_{sl}} = \frac{(t_2 - t_1)}{L_{sl}}(V_2 - nV_1) = \frac{\Delta_1 T_s}{L_{sl}}(V_2 - nV_1) \quad (11)$$

At the end of this State, the current of L_{sl} is the same as beginning of the cycle ($=I_1$).

Segment 2 $[t_2, t_3]$. In this Segment, the current in L_{sl} continues to decrease until zero when D_5 and D_8 freewheel is over, and Q_5 and Q_8 begin to conduct. The current in L_{sl} increases in the opposite direction until it reaches $-I_1$. The current ripple during this time interval is

$$\Delta I_{L_{sl}} = \frac{(t_3 - t_2)}{L_{sl}}(V_2 - nV_1) \quad (12)$$

Because of $t_3 - t_1 = (1-D)T_s$, in Segment 1 and Segment 2 the total current ripple in L_{sl} is

$$\Delta I_{L_{sl},2} = \frac{(1-D)T_s}{L_{sl}}(V_2 - nV_1) = I_{\max} + I_1 \quad (13)$$

The operation of Segment 3 through Segment 5 is symmetrical to Segment 0 through Segment 2.

In steady state, the average voltage across the leakage inductor must be zero. Note that segment 2 is symmetrical to segment 5; therefore, average inductor voltage in segment 1 and segment 2 should be zero:

$$DT_s(nV_1 + V_2) = \Delta_1 T_s(V_2 - nV_1) \quad (14)$$

Therefore, the relationship between input and output can be derived

$$V_2 = \frac{\Delta_1 + D}{\Delta_1 - D} nV_1 \quad (15)$$

Further, from (10) and (13), and using symmetry, it can be derived that

$$I_{\max} = \frac{T_s}{2L_{sl}} [V_2 - (1-2D)nV_1] \quad (16)$$

$$I_1 = \frac{T_s}{2L_{sl}} [(1-2D)V_2 - nV_1] \quad (17)$$

And

$$\begin{aligned} I_o &= \frac{1}{T_s} \left[I_1 (D + \Delta_1) T_s + \frac{1}{2} (I_{\max} - I_1) (D + \Delta_1) T_s \right] \\ &= \frac{1}{2} (D + \Delta_1) (I_1 + I_{\max}) \end{aligned} \quad (18)$$

Substitute (15) to (17) to (18), we can get

$$I_o = \frac{(D + \Delta_1)}{2L_{sl}} \frac{(1-D)T_s}{L_{sl}} (V_2 - nV_1) \quad (19)$$

Fig. 4. The operational States of the DC-DC converter in one period for the discontinuous mode.

4. Voltage Ripple

The capacitor current is the difference between the inductor current and the load current. We can calculate the output voltage ripple by assuming a constant load current. The capacitor current in continuous operation and “discontinuous operation” can be shown in Fig. 5.

$$\begin{aligned} I_C &= -(I_o + I_L) & 0 \leq t \leq DT_s \\ I_C &= I_L - I_o & DT_s \leq t \leq T_s \end{aligned} \quad (20)$$

&

$$I_{L,average} = \frac{I_o}{1-2D} \quad (21)$$

The voltage ripple is:

$$\begin{aligned} \Delta V_o &= \frac{DT_s}{2C} (I_1 + I_o + I_{\max} + I_o) = \frac{DT_s}{2C} (2I_{L,average} + 2I_o) \\ &= \frac{2DT_s I_o (1-D)}{C (1-2D)} \end{aligned} \quad (22)$$

In “discontinuous mode”:

$$\begin{aligned} I_C &= -(I_o + I_L) & 0 \leq t \leq DT_s \\ I_C &= I_L - I_o & DT_s \leq t \leq \Delta_1 T_s \\ I_C &= -(I_o + I_L) & \Delta_1 T_s \leq t \leq T_s \end{aligned} \quad (23)$$

The voltage ripple is

$$\begin{aligned} \Delta V_o &= \frac{DT_s}{2C} (I_1 + I_o + I_{\max} + I_o) \\ &= \frac{DT_s}{2C} (I_1 + I_{\max} + 2I_o) \end{aligned} \quad (24)$$

Since

$$\begin{aligned} I_{L,average} &= \frac{1}{T_s} \left[I_1 (DT_s + \Delta_1 T_s) + \frac{1}{2} (I_{\max} - I_1) (DT_s + \Delta_1 T_s) \right] \\ &= \frac{D + \Delta_1}{2} (I_{\max} + I_1) \\ &= \frac{D + \Delta_1}{2} \Delta I_{L_b} \end{aligned} \quad (25)$$

and

$$I_{L,average} = \frac{I_o}{1-2D} \quad (26)$$

Therefore

$$\Delta V_o = \frac{DT_s I_o}{C} \left[\frac{1}{(1-2D)(D+\Delta_1)} + 1 \right] \quad (27)$$

Fig. 5. The current ripple in the capacitor.

5. Simulation and Experiments

In order to validate the analytical analysis, a simulation model was setup in Simpler as shown in Fig. 6. The simulation results are shown in Fig. 7 for the continuous mode and Fig. 8 for the “discontinuous mode.”

Fig. 6. Simplorer model of the dual H-Bridge DC-DC converter.

Fig. 7. Simulated inductor current during continuous mode.

Fig. 8. Simulated capacitor current output voltage ripple during continuous mode.

Fig. 9. Simulated inductor current during "discontinuous" mode.

Fig. 11. Simulated capacitor current output voltage ripple during “discontinuous” mode.

We also have a test bench setup to validate the analysis and simulations as shown in Fig.11. The test is still in progress. Preliminary results have demonstrated functionality of the setup. Further test are needed to validate the different operation modes and verify the closed loop control.

Fig. 12. Experimental setup.

6. Conclusion

In this paper, we have analyzed the operation of the principle of a dual H-bridge bidirectional DC-DC converter. The mathematical analysis shows that there exist operation modes similar to the continuous mode and “discontinuous mode” of non-isolated boost converters. Modeling results validated the mathematical analysis. Experimental test is underway and further test results are expected to confirm the test results.

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Direct-Drive PM Wind Power Generation System with Simplified Power Converter Stages

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Abstract— This paper presents the study on the variable-speed direct-drive permanent magnet (PM) wind power generator systems with reduced power converter stages. The advantages and limitations of the proposed system were discussed. The design criteria and operation range of the PM generator for the reduced power converter stages were provided. The design rules for extending the variable speed range were discussed in detail. A prototype was designed and simulated to validate the proposed topology.

Index Terms — AC machines, AC-DC power converter, current locus, DC-AC power converter, direct-drive, generator, permanent magnet machines, PWM rectifier, variable speed wind generator (VSWG), wind power.

I. INTRODUCTION

Variable speed wind-power generator (VSWG) systems are becoming more and more attractive due to the many advantages of the systems [1]. For example, the annual energy capture of VSWG a system is at least 5% greater than that of a fixed-speed system [1]. The active and reactive power of VSWG systems can be easily controlled. There is no flicker problem to occur with variable-speed turbines, therefore there is less mechanical stress for the turbine blades. Rapid power fluctuations are scarce because the high inertia rotor acts as a flywheel. In addition, direct-drive permanent-magnet (PM) wind power generators allow the use of smaller pole pitch than do conventional generators so that higher efficiency can be achieved for the generator. Direct drive system also eliminate the need of gearbox so as to increase the system efficiency [1].

Direct-drive wind power generators are mostly synchronous machines. Therefore, the frequency and magnitude of the generator output changes with the wind turbine speed. In order to be connected to the utility grid, power converters must be inserted between the generator and the power grid. The most commonly used topology of power converter system for this purpose is shown in Fig. 1(a) [2-4]. There are two converters prior to the DC link in the system. One is an AC/DC converter, which converts the variable AC voltage of the generator output to a variable DC voltage. Another is a DC/DC converter which is used to maintain constant DC link voltage. The AC/DC converter is a simple passive rectifier [1]. The DC/DC converter is also unidirectional and can be either a buck or a boost converter depending on the base-speed chosen for the system.

Fig. 1 Topologies of direct-drive wind power generation systems. (a). Two-stage converter systems. (b). One-stage power converter systems.

A third power converter, the DC/AC inverter, converts the DC link voltage to AC voltage with frequency and voltage suitable to be connected to the power grid. Because there are two converters prior to the DC link, it is referred to as “two-stage power converter system.”

The unidirectional power flow of the converters prior to the DC link prevents the use of grid power and PM generator to start the wind turbine system. If the wind turbine needs to be started by the PM machine, as required by most direct-drive wind power generation systems, then both the AC/DC converter and the DC/DC converter need to be bidirectional [5].

In this paper, a reduced power converter stage system is proposed as shown in Fig. 1(b). In this topology, the former two-stage converters are replaced with one power electronics converter. The DC/DC converter is eliminated. Hence it is a one-stage converter system which can simplify the system and reduce the power converter losses. Besides the simplified structure, this topology can also help start the wind turbine system using the PM generator. At the breezing condition, it is difficult to start the wind turbine because of the existence of detent torque and large inertia of the direct-drive PM generator. The self start feature is a desirable feature for large wind power generator systems.

In the one stage converter system, the PWM rectifier will function as a boost converter to keep the DC link voltage

constant. The system parameters will affect the adjustable speed range and system efficiency.

Although direct-drive PM generator designs have been extensively studied, the focus is primarily on the two-stage converter systems [6-10]. One-stage direct-drive PM wind power generation systems have not been studied in detail [11-13].

In this paper, the feasibility and design criteria for the direct-drive PM wind power generator with reduced power converter stages will be discussed. A prototype is designed and simulated to validate the proposed topology. It is shown that the one-stage converter system provide many advantages but impose great challenges to the design of PM generators with regard to the system performance and operating range.

II. LOCUS OF PM WIND GENERATOR SYSTEM WITH ONE-STAGE POWER CONVERTER

In the conventional two-stage PM wind generator systems, the wind-turbine cut-in speed (minimum speed) or the cut-off speed (maximum speed) can be chosen as the base speed for the PM generator [1]. If the cut-in speed is chosen as the base speed, then at speeds above the base speed, the constant DC link voltage is maintained by a DC/DC buck converter. If the cut-off speed is chosen as the base speed, then at speed below the base speed, the constant DC link voltage is maintained by a DC/DC boost converter.

In direct-drive PM wind generator systems with one-stage power converter, the base speed is between the wind turbine cut-in speed and cut-off speed. Consequently, at speed below the base speed but above the cut-in speed, the output voltage of the PM generator will be boosted to the rated DC link voltage by the PWM rectifier. At speed above the rated speed but below the cut-off speed, the generator enters into flux weakening region to maintain constant DC link voltage. In addition, beyond the base speed, the DC/AC inverter can also be controlled by reducing the amplitude modulation ratio to maintain voltage output suitable for the grid connection.

If the maximum power tracking is desired for the cut-off speed, then the cut-off speed will be designed as the rated speed.

There are many factors that affect the conditioning process and variable speed range. In order to maintain the DC link voltage constant and achieve high efficiency operation in the full speed range, the generator and the power converter must satisfy certain design criteria.

The voltage and flux-linkage equations of a PM generator in the dq coordinate can be written as:

$$\begin{cases} v_d = \frac{d}{dt}\psi_d - \omega \cdot \psi_q - R_1 \cdot i_d \\ v_q = \frac{d}{dt}\psi_q + \omega \cdot \psi_d - R_1 \cdot i_q \end{cases} \quad (1)$$

$$\begin{cases} \psi_d = L_d \cdot i_d + \psi_{PM} \\ \psi_q = L_q \cdot i_q \end{cases} \quad (2)$$

where

v_d, v_q — stator voltage along d-axis and q-axis windings;

i_d, i_q — stator current along the d-axis and q-axis windings;

$\psi_d, \psi_q, \psi_{PM}$ — flux linkage of the stator d-axis, q-axis windings and PM pole;

L_d, L_q — synchronous inductance along the d-axis and q-axis;

R_1 — resistor of the stator windings

ω — the rotor speed in rad/s.

Under steady state conditions, the voltage equations can be rewritten as:

$$\begin{cases} v_d = -\omega \cdot L_q \cdot i_q - R_1 \cdot i_d \\ v_q = \omega \cdot L_d \cdot i_d + \omega \cdot \psi_{PM} - R_1 \cdot i_q \end{cases} \quad (3)$$

When the winding resistance R_1 is neglected, the RMS value of the voltage vector can be written as

$$V = \sqrt{V_d^2 + V_q^2} = \sqrt{(-\omega L_q i_q)^2 + (\omega L_d i_d + \omega \psi_{PM})^2} \quad (4)$$

It can be seen from (4) that the generator output voltage will vary with the turbine speed. At low turbine speed, the output voltage of the generator should be boosted to the rated DC link voltage by control of the PWM rectifier. Otherwise the wind power can not be fed into the grid.

Assuming that the rated DC link voltage is V_r , the rated fundamental phase voltage of the Y connected generator is:

$$V_{ph-rated} = \frac{V_r}{\sqrt{6}} \quad (5)$$

In the d-q coordinate system, the rated voltage should be

$$V_{dq-rated} = \sqrt{3} \cdot V_{ph-rated} = \frac{V_r}{\sqrt{2}} \quad (6)$$

Substituting the variable V in (4) with $V_{dq-rated}$, the following relationship can be obtained:

$$(i_d + \frac{\psi_{PM}}{L_d})^2 + (\frac{L_q}{L_d} \cdot i_q)^2 = (\frac{V_{dq-rated}}{\omega \cdot L_d})^2 \quad (7)$$

For the surface mounted PM machine, the inductances along d-axis and q-axis are almost the same, i.e., $\frac{L_q}{L_d} = 1$.

Therefore, the locus of (7) is a circle, with the center point at $(-\frac{\psi_{PM}}{L_d}, 0)$, and radius $(\frac{V_{dq-Rated}}{\omega \cdot L_d})$. The voltage locus is shown in Fig. 2 under constant DC link voltage.

Because of the limitation of the power devices, current should also be limited in a given range

$$i_d^2 + i_q^2 = i_{dq-lim}^2 \quad (8)$$

where $i_{dq-lim} = \sqrt{3} \cdot i_{ph-lim}$ is the maximum current that the power converter can provide.

The current limitation locus described by (8) is also a circle, with the center at the original as shown in the Fig. 2.

The intersection area of the voltage and current loci are the available operation range of the system. It can be concluded that from the loci that:

- The optimal point is point A on the q-axis. In this condition, all the available current will be used for torque capturing. Therefore, this point should be designed as the rated operating point for the wind generation system.
- As the speed increases or decreases, the d-axis current needs to be controlled accordingly in order to maintain maximum power operation. For example, when the speed decreases from ω_3 to ω_1 , the d-axis current needs to be changed from point B to C, and the polarity of the current is also reversed. The d-axis current changes from field-weakening to field-strengthening.
- Because of the current limitation, the turbine speed range for keeping constant DC link voltage is limited. The speed range which can be controlled to maintain the constant DC link voltage is only the intersection of these two loci.

Therefore, in order to obtain a constant DC link voltage for a wide speed range, both the power converter and the PM generator parameters needs to be designed properly.

Fig. 2 Voltage and Current locus of PM motor used for direct-drive wind power generator.

III. DESIGN CRITERIA OF THE PM GENERATOR

Under the condition of $L_d = L_q = L$, the following relationship can be derived from (7):

$$i_s^2 + 2i_d \cdot \frac{\Psi_{PM}}{L} + \left(\frac{\Psi_{PM}}{L}\right)^2 = \left(\frac{V_{dq-rated}}{\omega \cdot L}\right)^2 \quad (9)$$

Define the characteristic current as

$$I_{ch} = \frac{\Psi_{PM}}{L} \quad (10)$$

then at the rated speed ω_N , equation (9) can be re-written as

$$i_{lim}^2 + 2i_{dN} \cdot i_{ch} + (i_{ch})^2 = \left(\frac{V_{dq-rated}}{\omega_N \cdot L}\right)^2 \quad (11)$$

At the lowest speed (cut-in speed) ω_1 , equation (9) can be expressed as

$$i_{lim}^2 + 2i_{d1} \cdot i_{ch} + (i_{ch})^2 = \left(\frac{V_{dq-rated}}{\omega_1 \cdot L}\right)^2 \quad (12)$$

Define the variable speed ratio N as:

$$N = \frac{\omega_N}{\omega_1} \quad (13)$$

Divide (11) by (12), the following relationship can be obtained

$$\frac{i_{lim}^2 + 2i_{dN} \cdot i_{ch} + i_{ch}^2}{i_{lim}^2 + 2i_{d1} \cdot i_{ch} + i_{ch}^2} = \left(\frac{\omega_1}{\omega_N}\right)^2 = \left(\frac{1}{N}\right)^2 \quad (14)$$

Therefore, the field strengthening current at the cut-in speed should be,

$$i_{d1} = \frac{(N^2 - 1) \cdot (i_{lim}^2 + i_{ch}^2)}{2 \cdot i_{ch}} + N^2 \cdot i_{dN} \quad (15)$$

From (11), the following relationships can also be obtained:

$$i_{lim}^2 + i_{ch}^2 = \left(\frac{V_{dq-rated}}{\omega_N \cdot L}\right)^2 - 2i_{dN} \cdot i_{ch} \quad (16)$$

Substitute (16) to (15), the d-axis field strengthening current I_{d1} at the cut-in speed can be derived

$$i_{d1} = (N^2 - 1) \cdot \left(\frac{V_{dq-rated}}{\omega_N}\right)^2 \frac{1}{L \cdot \Psi_{PM}} + i_{dN} \quad (17)$$

where

$$i_{dN} = \frac{1}{i_{ch}} \cdot \left(\left(\frac{V_{dq-rated}}{\omega_N L}\right)^2 - (i_{lim}^2 + i_{ch}^2) \right) \quad (18)$$

In order to obtain the maximum power point track (MPPT) at the rated speed, the following relationship should be observed:

$$\begin{cases} i_{dN} = 0 \\ i_{qN} = i_{dq-lim} \end{cases} \quad (19)$$

This is the point A shown in Fig. 2.

Hence in order to keep constant DC link voltage at the cut-in speed ω_1 , the d-axis current will be

$$i_{d1} = (N^2 - 1) \cdot \left(\frac{V_{dq-rated}}{\omega_N}\right)^2 \frac{1}{L \cdot \Psi_{PM}} \quad (20)$$

The operating speed range:

$$N = \sqrt{i_{d1} L \cdot \Psi_{PM} \left(\frac{\omega_N}{V_{dq-rated}}\right)^2 + 1} \quad (21)$$

It can be seen from (20) and (21) that:

- In order to obtain a wide speed range, large field strengthening current i_{d1} is needed.
- Because of the current limitation of the power converter, there is a limitation for the variable speed range to keep the DC link voltage constant. In order to achieve a wider speed range, a higher current rating is needed for the power converter.
- Below the rated speed, the generator enters into field strengthening region. The power can be fed back to the grid is reduced due to the fact that portion of the available current is used for field weakening.
- The overall speed range of the system can be extended to the field weakening region to cover speed above the

rated speed but less than the cut-off speed. The output power is reduced even though the turbine speed is higher.

IV. DESIGN AND SIMULATION OF THE PROPOSED PM GENERATOR WITH ONE-STAGE POWER CONVERTER

Based on the principles discussed above, a prototype for direct-drive wind power generator is designed with one stage power converter system. It is a surface-mounted direct-drive PM generator. The geometry and its flux distributions are shown in Fig. 3. The rating, main dimensions and parameters are shown in Table I and II respectively.

A multi-pole rotor, 44 poles, was chosen for the direct-drive generator design. The slot/pole ratio is chosen to be 42/44. The Slot-per-phase per-pole (SPP) is very small $SPP=7/22$.

Therefore, with this slot/pole ratio, concentrated and fractional winding is used. There are some advantages with this design such as reduced winding end-turn length, which can reduce the copper loss; and reduced cogging torque. The fractional slot design can increase the winding inductance, which is in favor of extending the variable speed range with small field strengthening current [8].

The simulation model of the proposed wind power generator system is shown in Fig. 4 and was simulated using Simplorer, a software package from Ansoft. In this model, state machine is used to control the switching of the IGBTs. The wind turbine output is given as T_{turbine} , which is the input variable to the direct-drive PM generator.

Fig. 3. The geometry and its flux distributions of the prototype design.

TABLE I. RATED DATA OF THE PM GENERATOR

Parameter	Rating	Unit
Rated power	22	kW
Rated speed	200	rpm
Rated Torque	1000	Nm
Cut-in speed (minimum speed)	100	rpm
Cut-off speed (maximum speed)	300	rpm
Rated DC voltage	310	V

TABLE II. MAIN DIMENSIONS AND PARAMETERS OF THE PM GENERATOR

Parameter	Value	Unit
Stator Outer Diameter	450	mm
Stack length	310	mm
Number of poles	44	
Num of Slots	42	
Rotor inertia	2.209	kg.m ²
Flux linkage	0.328	Wb
EMF coefficient (K_e)	0.51	V/rpm
Ld	2.79	mH
Lq	2.78	mH

Fig. 4. Simulation model of the proposed wind generator system in Simplorer.

TABLE III. COMPARISON OF VOLTAGES AT THE DC SIDE

Speed (rpm)	DC Link Voltage (V)	
	Diode rectifier	PWM rectifier
305	350	350
210	208	302
150	170	305
100	124	300

The grid phase voltage is 110V. Therefore, the voltage at the DC side is:

$$V_{DC-rated} = \sqrt{2} \cdot \sqrt{3} \cdot V_{grid-phase} \quad (20)$$

In the simulation, the rated DC link voltage is assumed to be 300V. The simulated DC voltages at different speeds are shown in Table III. As a comparison, the output voltage with passive diode rectifier is also shown in Table III. The simulated waveforms for 210rpm, 150rpm and 100rpm are shown in Figs. 5-7 respectively.

It can be seen that at lower speeds, the DC link voltage can be maintained constant by control of the PWM rectifier. In order to keep constant DC link voltage, as the speed decreases, the d-axis current needs to be increased accordingly. For example, when speed decrease from 210rpm to 100rpm, the d-axis current increase from 13.8A to 58.5A, as shown in Fig. 5.

V. CONCLUSIONS

This paper presented the analysis, design and simulation of the direct-drive wind PM generator with one-stage PWM rectifier control system. It can be concluded that:

Fig. 5. Simulated waveforms of the prototype with torque at 1000Nm and speed at 200rpm. Upper: DC link voltage; middle: turbine/generator speed; lower: d-axis current.

Fig. 6. Simulated waveforms of the prototype with torque at 500Nm and speed at 150rpm. Upper: DC link voltage; middle: turbine/generator speed; lower: d-axis current.

Fig. 7. Simulated waveforms of the prototype with torque at 150Nm and speed at 100rpm. Upper: DC link voltage; middle: turbine/generator speed; lower: d-axis current.

- There are many advantages for the one-stage, direct-drive wind generator. But with the limitation of the voltage on the DC side and current of the power device, tight design criteria for the generator must be imposed.
- A design with concentrated, fractional slot winding and multi-pole PM generator validated the design.
- Simulation of the generator system provided a good

validation for the design criteria presented in the paper.

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Design and Testing of Silicon Carbide JFET Based Inverter

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Abstract— This paper presents the design and testing of a high frequency, high efficiency inverter using silicon carbide (SiC) JFET power module. A rugged negative voltage gate drive circuit is used to solve the normally on problem of JFET devices and avoid the bridge shot-through during power on or power off. The circuit can provide over-voltage protection, over current protection and over temperature protection circuits to ensure the safe operation of the SiC JFET module and the resultant inverter system. The simulation and measurement results show that SiC JFETs have short turn-on and turn-off times, which will result in lower switching losses than silicon (Si) IGBTs. The low on-resistance in SiC JFETs will result in lower conduction losses. The experiment results of a 1kW SiC JFET-based inverter showed 3% efficiency improvement by a SiC JFET-based inverter over a Si IGBT- based inverter.

Keywords-Silicon Carbide, SiC JFET, inverter, gate drive circuit.

I. INTRODUCTION

Silicon carbide (SiC) semiconductor has the characteristics of wide bandgap (3.0eV for 6H-SiC), higher saturation velocity (2×10^7 cm/s), high thermal conductivity (3.3-4.9 W/cmK), low on resistance ($1 \text{ m}\Omega/\text{cm}^2$) and high breakdown electric field strength (2.4MV/cm) [1-3]. Therefore, SiC power devices will have the advantages of larger current carrying capability, higher voltage block capability, high operating temperature, and less static and dynamic losses than traditional silicon (Si) power switches. In addition, SiC power devices can operate at higher switching frequencies. Therefore, in a inverter system using SiC power devices, the size of its passive components (inductor and capacitor) can be reduced due to the higher frequency operation, so does the associated heatsinks due to lower losses generated as compared with a conventional Si system. At the present time, it is still difficult to produce SiC MOSFET. SiC JFET, on the other hand, is easier to be manufactured and currently is at engineering stage that is being commercialized. As the manufacture technique improves and its mass production can be realized, it is anticipated that there will be more SiC JFET power switches used in power electronic systems.

SiC JFETs are “normally-on” devices [4]. For SiC JFETs to be incorporated in the presently used power converter system designs, there are two possible solutions. One is to use negative voltage to turn it off. For example [4], a flyback transformer was used to generate the negative gate drive voltage to turn off the SiC JFET. This technique is suitable for DC/DC converters with narrow variation of duty cycle. The other solution is to use a SiC JFET plus a low on-resistance Si MOSFET cascade to form a normally off controlled SiC switch [5]. In this design, the gating circuit same as conventional MOSFETs can be used in the

inverter applications like normal MOSFETs. However, the introduction of the additional Si MOSFET will add the system cost and bring additional losses.

This paper presents the development of a high-frequency, high-efficiency inverter using SiC JFET modules. In this system, a negative gate drive voltage is used to turn off the SiC JFET, and the gate drive circuit gets power from the DC rail to ensure the safe operation of SiC JFET devices. In addition, the gate driver circuit is optical-isolated and the control logic is the same as traditionally normally off devices. This design enables the integration of the SiC JFET, the driver circuit and the protect circuit into one smart power module. The simulation and experiment results of a SiC JFET inverter and an IGBT inverter demonstrated the low on-state voltage drop and high switching speed prospects of SiC power JFET. The SiC JFET Module inverter using a SiC JFET module shows more than 3% higher efficiency than the new-generation Si IGBT based inverter in wide switching frequency ranges.

II. CIRCUITS DESIGN

The design of this SiC JFET inverter is shown in Fig. 1. The main circuit is similar to a traditional inverter circuit, which consists of the soft start relay, EMI filter, bulk capacitor, SiC JFET module (six packed SiC JFET and anti-parallel SiC diode), current/voltage sensing circuit and protection circuit. The protection circuit includes three-phase over current, DC bus over voltage, over temperature, driving pulse short-through lock, fault LED display and auto reset circuits. The control signals from TMS320F2407 or dSPACE DS1104 system is sent to the protection and driver board to gate the SiC JFET module.

For the SiC-JFET-Module-based inverter system, one important and special issue is the gate drive circuit design. Because of the “normally on” feature of SiC JFET, the SiC JFET turns on at gate voltage close to 0V. A negative voltage, usually -24V, is necessary to turn off the SiC JFET.

The negative gate drive voltage must block the module to prevent the shot-through of the bridge when system is powered up. This implies that negative gate voltage must be applied before the DC-rail voltage is applied to the SiC JFETs. In addition, the negative gate voltage should also force the SiC JFET devices off when the inverter is powered off and the discharge of bulk capacitor is not initiated yet.

The gating logic in Fig. 2 is similar to that of a conventional inverter. When the PWM signal from the digital controller is high, then the gating voltage is equal to $V_{CC}(5V)$ and the SiC JFET turns on. When PWM signal from the digital controller is low, then the gating voltage is equal to $V_{SS}(-24)$, and the SiC JFET turns off.

Fig. 1. SiC-JFET based inverter system

Fig. 2. Gate drive circuit and measured gate waveforms. (a) SiC JFET gate drive circuit, (b) gate drive waveforms

In this paper, the DC rail voltage is used to power the driver circuit as shown in Fig. 2(a). This design can avoid the unexpected breakthrough of SiC JFETs. At startup, the DC rail voltage is applied to the gate drive circuit before the startup relay closes. The relay only closes once the negative gate voltage is generated and applied to the gates of SiC JFETs.

The gate driver circuit is designed to be optical-isolated, so that it is convenient to integrate this driver circuit later into the power module, and make the application of SiC JFET more feasible with the normally-on issue. Fig. 2(b) shows the measured PWM waveform from the digital controller, and the gate drive circuit.

III. SIMULATION AND LOSS ANALYSIS

Before the experiment, a Pspice model of SiC JFET and SiC JFET-based circuit was established as shown in Fig. 3. Simulation parameters are from SiC JFET die manufacturing company and test results [6]. Each die has a maximum drain-source voltage great than 1200V (@Q25°C, $I_{dss} < 2\text{mA}$), maximum drain-source leakage current less than 0.4 mA (@Q25°C, 400 V), 7 amperes rated drain-source current, and $R_{on} < 0.25\text{ Ohm}$ (@25°C). There are 2 to 4 dies parallel to form one switch unit.

Figs. 4-5 show the simulated switching waveforms of Si IGBT and SiC JFET. The turn-on time of the SiC JFET is about 50ns while the turn-on time of IGBT is about 100ns. The turn-off time of the SiC JFET is about 50ns while the one of IGBT is about 100ns with a 0.5us tail current time.

To calculate the losses of the SiC JFET inverter with sinusoidal output, assume the sinusoidal current lagging the sinusoidal output voltage an angle of θ , as shown in Fig. 5.

The angle corresponds to a constant power factor. Similar to the loss calculation of conventional hard switching inverter [7-8], the conduction and switching losses of the SiC JFET and SiC diode can be derived as following.

Fig. 3. SiC JFET inverter simulation circuit

(a)

(b)

Fig. 4. Turn-on waveforms. (a) IGBT (b) SiC JFET

A. Conduction Loss

For large ratio between carrier frequency and modulation frequency, the duty cycle of the power switch and anti-parallel diode function are:

$$\begin{cases} D_s(\alpha) = \frac{1}{2} [1 + m \sin(\alpha + \theta)] \\ D_d(\alpha) = \frac{1}{2} [1 - m \sin(\alpha + \theta)] \end{cases} \quad (1)$$

α is the phase angle of current waveform and m is modulation index.

The power switch and diode conduction loss within any angle α is:

$$\begin{cases} P_s(\alpha) = [I_M \sin(\alpha) \cdot V_{s(on)}(I) \cdot D_s(\alpha)] \\ P_d(\alpha) = [I_M \sin(\alpha) \cdot V_{d(on)}(I) \cdot D_d(\alpha)] \end{cases} \quad (2)$$

(a)

(b)

Fig. 5. Turn-off waveforms. (a). IGBT (b). SiC JFET

where

$$\begin{cases} V_{s(on)}(I) \approx I_M \sin(\alpha) \cdot R_{s(on)} \\ V_{d(on)}(I) \approx V_f + I_M \sin(\alpha) \cdot R_{d(on)} \end{cases} \quad (3)$$

Each device's averaged conduction time is only one half of the switching period, so

$$P_{avg} = \frac{1}{2\pi} \int_0^\pi P(\alpha) d\alpha \quad (4)$$

Therefore the conduction loss of SiC JFET and the SiC diode can be obtained:

$$\begin{cases} P_{s(con)} = \left[(I_M)^2 \cdot R_{s(on)} \cdot \left(\frac{\sqrt{3}}{8\sqrt{\pi}} + \frac{m}{3\pi} \cos \theta \right) \right] \\ P_{d(con)} = \frac{1}{2} I_M \cdot V_f \left(\frac{1}{\pi} - \frac{m}{4} \cos \theta \right) + (I_M)^2 \cdot R_{d(on)} \cdot \left(\frac{\sqrt{3}}{8\sqrt{\pi}} - \frac{m}{3\pi} \cos \theta \right) \end{cases} \quad (5)$$

Fig. 6. Current and voltage waveforms the inverter output.

Fig. 7. V_{ce} and I_c waveform during switching.

B. Switching Loss:

To calculate the switching loss, the current and voltage are assumed to vary linearly during the switching on and off as shown in Fig. 7. Because the SiC diode has nearly no reverse recovery current, the switch has no turn-on loss caused by diode reverse current and has no reverse recovery loss.

From Fig. 7, the turn-off loss is:

$$E_{off} = V \cdot I_o \cdot t_{off} / 2 \quad (6)$$

The average turn-off loss in the whole period is:

$$P_{off} = f_s \cdot \frac{1}{\pi} \int_0^\pi E_{off} d\alpha = \frac{V \cdot I_M \cdot t_{off} \cdot f_s}{\pi} \quad (7)$$

Similarly, the turn-on loss is:

$$E_{on} = V \cdot I_o \cdot t_{on} / 6 \quad (8)$$

The average switching on losses in one period is:

$$P_{on} = f_s \cdot \frac{1}{\pi} \int_0^\pi E_{on} d\alpha = \frac{V \cdot I_M \cdot t_{on} \cdot f_s}{3\pi} \quad (9)$$

For the 1kW inverter, the calculated loss and efficiency curve of SiC JFET module and the 3rd generation Si IGBT module are shown in Table I. Because the SiC has very low on-resistance, and short switch on/off time, the conduction loss and switching losses of SiC JFET are much lower than that of Si IGBT.

By adding losses of other circuit components (driving circuit, relay, power supply, etc.), the efficiency of SiC JFET inverter and Si IGBT inverter at different switching frequency can be calculated, as shown in Fig. 8. It can be seen that the SiC JFET inverter has much higher efficiency than Si IGBT inverters and is more suited for high frequency applications.

TABLE I. CALCULATED LOSSES OF SiC JFET MODULE VS. 3RD GENERATION Si IGBT MODULE AT $V_{DC}=200V$, $P=1KW$ (W)

	20kHz		50kHz		100kHz	
	SiC JFET	Si IGBT	SiC JFET	Si IGBT	SiC JFET	Si IGBT
P_{Scond}	2.1	10.5	2.1	10.5	2.1	10.5
P_{Dcond}	1.3	7.3	1.3	7.3	1.3	7.3
$P_{S on}$	0.5	1.2	1.25	3	2.5	6
$P_{S off}$	3.1	10.1	7.7	25.25	15.5	50.5
$P_{D reverse}$	0	2.2	0	5.5	0	11

Fig. 8. Calculated efficiency of SiC JFET module vs Si IGBT module.

IV. EXPERIMENTAL RESULTS

The 1kW, 200V inverter was built and tested with both Si IGBT and SiC JFET as shown in Fig. 9. Test results of the three-phase inverter prototype using SiC JFET (with anti-parallel SiC diode) validated the simulation and calculations.

The circuit for measuring the switching on/off times is shown in Fig. 10, and the inverter measurement circuit is shown in Fig. 11. Yokogawa PZ4000 power analyzer is used to record and analyze the efficiency and output current quality of the inverter. The load connected to the inverter is a three-phase induction machine rated at 3 Hp, 60Hz, 1800 rpm, 208V, and 10.8A.

Fig. 9. SiC inverter assembly

Fig. 10. Circuit measuring switching times

Fig. 11. Circuit for measuring inverter efficiency

(a)

(b)

Fig. 12. Measured turn-on waveforms. (a) SiC JFET without anti-parallel diode. (b) SiC JFET with anti-parallel diode.

Figs. 12 to 14 show the experimental results of SiC JFET with and without anti-parallel diode. The turn on, turn off and reverse recovery current waveforms are shown. The tested turn-on time of SiC is approximately 80ns and turn off time is approximately 100ns. The turn-on time is mainly attributed by the test circuit parameters [9].

The parasitic diode of SiC JFET has a very big reverse recovery current when no anti-parallel diodes present. When anti-parallel SiC diode is in place, the reverse recovery current was greatly improved. Therefore, it is necessary to have SiC fast recovery anti-parallel diode with SiC JFET in high performance applications.

For the purpose of comparison, the switching waveforms of Si IGBTs using the same gating circuitry are shown in Fig. 15. It can be seen that the SiC JFET has much smoother switching characteristics than Si IGBT. Both switching on time and switching off time of Si IGBT are longer than that of SiC JFET.

Fig. 16 shows the experimental efficiency of SiC JFET-based inverter with anti-parallel SiC diode and the 3rd generation Si IGBT-based inverter. The SiC JFET inverter shows 94% efficiency at 30kHz switching frequency operation at 1kW, 150V_{DC}, while the Si IGBT-based inverter only achieved 90% efficiency at the same switching frequency.

(a)

(b)

Fig. 13. Measured turn-off waveforms. (a) SiC JFET without parallel diode. (b) SiC JFET with parallel diode.

Fig. 14. Reverse recovery current waveforms. (a) SiC JFET with parasitic diode. (b) SiC JFET with anti-parallel diode.

Fig. 15. Switching waveforms of Si IGBT. (a) turn-on waveforms. (b) turn-off waveforms.

V. CONCLUSION

This paper discussed the design and experiments of SiC JFET based inverter, with special focus on the gate drive circuit design. In this design, the DC rail voltage is used to power the gate drive circuit and to interlock the relay (soft-start) that prevents the power-up of the SiC module before negative gating signal is applied at the gates. The combination of negative gate voltage and the interlock mechanism will prevent the breakthrough of SiC JFET modules that are normally-on device.

The measurement shows significant reduction in switch-on/off time and on-state resistance in SiC JFET modules as compared to conventional IGBT modules. The simulation and experiments on the 1kW 3-phase sinusoidal SiC inverter show significant efficiency improvement over conventional IGBT inverters over a wide range of switching frequencies.

Since higher switching frequency can be easily achieved in SiC JFET based inverters, a considerable

Fig. 16. Inverter efficiency curves of SiC JFET vs. Si IGBT

reduction of the size of passive components in inverters can be also anticipated.

In the first phase of test used SiC JFETs without the anti-parallel diodes. It relied on the parasitic diodes of the JFETs to conduct reverse current. In the test, it showed large reverse recovery current. Then the inverter is built with SiC JFETs that has external anti-parallel diodes and at a large power rating (14A). Approximately 1% of efficiency improvement was observed in the test by the inverter that is designed with anti-parallel diodes.

High temperature operation up to 300°C has also been demonstrated for SiC modules. In the next phase of study, the operating temperature of the SiC inverter system will be tested. Higher power rating up to 5kW and later 50kW will be achieved by using parallel connected SiC JFETs.

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PEM Fuel Cell Stack Characterization and its Integration in Simulating a Fuel Cell Powertrain

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ABSTRACT

Fuel cell based powertrains are considered as potential candidates for future vehicles. Modeling of vehicle powertrains, using a combination of components and energy storage media, are widely used to predict vehicle performances under different duty cycles.

This paper deals with performance analysis of a light-duty vehicle comprised of a PEM fuel cell stack, in combination with different energy storage systems using Powertrain Simulation Analysis Toolkit (PSAT). The performance of the stack was characterized by experimental data on a smaller PEM stack and was used in the simulation. The stack data was collected at controlled loading and thermal parameters. Three energy storage systems are considered in the analysis: nickel metal hydride battery storage, lithium-ion battery storage and ultra capacitor energy storage.

The simulation results were analyzed for comparative evaluations and to optimize the performance of the fuel cell powertrain configurations. The study shows that a combined energy storage system, involving batteries and ultra-capacitors, provide vehicle performance equivalent to the combustion engine powered vehicle. The size of the fuel cell size also impacts predicted fuel economy and vehicle acceleration time. The impact of various energy storage system technologies on simulated vehicle performance is discussed in the paper.

INTRODUCTION

A Hybrid Electric Vehicle (HEV) combines two sources of energy, and has been introduced in automotive market in an effort to improve fleet fuel economy and possibly reduce environmental impact of combustion engines.

Hybrid electric vehicles combine a conventional vehicle drivetrain with subsystems commonly found in an electric vehicle. In this type of vehicle, the internal

combustion engine is generally augmented by an electric motor and electric energy storage system. In a fuel cell hybrid electric vehicle (FCHEV) the combustion engine is replaced by a fuel cell stack. The stack harnesses electrochemical energy when hydrogen and oxygen react in the cells. Additional energy storage system (ESS) is generally needed to address fuel cell stack (FCS) operating characteristics and vehicle transients. Fuel cells have high efficiency and, by themselves, produce water as byproduct and hence are non-polluting devices. Unlike combustion engines, fuel cells produce no noise although the additional components needed to operate the stack are not noiseless. Fuel cells have the capability of producing electrical energy as long as the fuel and the oxidant are supplied to the electrodes and operating conditions are appropriate. Fuel cell hybrid electric vehicles have several advantages over fuel cell powered vehicles without ESS:

- Improved fuel economy due to energy recovery from regenerative braking.
- Improved efficiency by operating the stack at part load through ESS load sharing during transient demands like rapid acceleration
- Possible cost benefits through the right degree of hybridization. Downsizing the stack, and increasing the size of the ESS could help reduce the overall system cost by reducing the FCS balance of plant costs

The main systems of a fuel cell vehicle consist of:

- The fuel processing and/or storage system
- The fuel cell stack where the hydrogen gas and air react to produce electrical power and heat
- Power electronics to convert the fuel cell power to the required type of power
- Energy storage systems (batteries or capacitors)
- The electric drivetrain system (motors, controls, etc.)

A successful automotive fuel cell system is desired to have operational and performance characteristics similar to those of the modern day internal combustion engine based vehicles. System safety, fuel efficiency, ease of use and maintenance are some of the other key requirements. The concept of FCHEV is not new. Past investigations have focused on storage media with default characteristics of the fuel cell [1,2]. The Fuels and Energy Conversion Laboratory at the University has been conducting research and development on proton exchange membrane (PEM) FCS as part of advancing fuel cell technology for vehicles and distributed power generation and to better understanding the complexities involved fuel cell based automotive powertrains.

Figure 1. Cell Polarization Curve

A laboratory version of PEM fuel cell stack (Plug Power) was used in the investigation. The stack was operated at different thermodynamic and flow conditions to characterize stack performance. The results from the tests were scaled and incorporated into Powertrain System Analysis Toolkit or PSAT [3] based fuel cell model. The model was applied to a medium-sized sport utility vehicle (SUV). Different energy storage devices were used in the simulation for various drive cycles. This paper deals with results and analyses of a FCHEV powertrain that is based on experimental FCS characterization and several energy storage systems.

FUEL CELL STACK CHARECTERIZATION

A PEM fuel cell stack (Plug Power) with 8 cells, each with an effective area of 252 cm², was used in the experiments.

Table 1 : PEMFC test conditions

Hydrogen temperature (C)	50 -75
Oxidant gas (air) temperature (C)	50-75
Hydrogen relative humidity, %	70 -100
Air relative humidity, %	70 - 100
Stack operating pressure, kPa	Atm.

The stack was operated on compressed hydrogen and

air and at a pressure slightly higher than atmospheric. A series of tests were conducted to characterize polarization curves and stack efficiency at various fuel and air stoichiometry. Figure 1 shows cell polarization curve and Figure 2 shows average stack efficiency, based on hydrogen heating value, when the fuel and air

Figure 2. Stack Efficiency

temperatures were maintained at 70 C and gas relative humidity at 100%. Best efficiency was realized when the hydrogen stoichiometry was 1.0. Although hydrogen stoichiometry of $\lambda = 1.0$ resulted in high efficiency, effective operation of the stack required that hydrogen flow rate be slightly higher to ensure its uniform distribution in all the cells.

The effects of fuel and air temperatures and their relative humidity on stack efficiency are shown in Figure 2. Not significant differences in efficiency were observed for gas temperatures in the range of 50-70C and relative humidity between 70 - 100%. But, 70C temperature and a relative humidity of 90-100% produced marginally better results over most of the range, as shown in Figure 3. The steady state operating efficiencies, with hydrogen and air stoichiometry of $\lambda = 1.2$ and 2.5, respectively, at 70C and relative humidity of 100, were incorporated in the PSAT fuel cell model and were used in the simulations. Fuel cell stack loading under transient conditions revealed a short delay in FC response or a small additional drop in stack voltage which was recovered within a few seconds. Other than the default data, the experimental observations on transients were not separately modeled in PSAT modifications. The following assumptions were made in the fuel cell model:

- Maximized steady state stack operation
- Uniform stack temperature of 70C
- Ideal gas behavior of the reactant gases
- Uniform stack humidity of 100%
- No chemical kinetics limitations.

POWER and ENERGY STORAGE

The computation for selecting the various powertrain components were initially made on expected performance of a similar vehicle. The vehicle selected for the analysis was a sport utility vehicle (SUV) with specifications given in Table 2.

Table 2: Vehicle data for simulation

Mass 'm' (kg)	2200
Frontal Area 'A' (m ²)	2.686
Coefficient of Drag, 'C _d '	0.417
Coefficient Of Rolling Resistance, 'C _{rr} '	0.01

The power requirements were based on vehicle requirements for acceleration, grade climbing and resistance due to aerodynamic drag and rolling resistance. The computations of power requirements were made using equations (1) – (5):

$$P_{road} = P_{roll} + P_{hill} + P_{aero} + P_{accel} \quad \dots (1)$$

$$P_{roll} = m.V.g.C_{rr}.cos\theta \quad \dots (2)$$

$$P_{hill} = m.g.V.sin\theta \quad \dots (3)$$

$$P_{aero} = 0.5 \rho.A.V^3.C_d \quad \dots (4)$$

$$P_{accel} = dE_{kinetic}/dt = m.V.dV/dt \quad \dots (5)$$

Table 3: Vehicle and FC specifications/requirements

Target 0 –100 km/h acceleration (s)	10
Speed at 6.5% grade (km/h)	90
Maximum speed (km/h)	165
Calculated peak power (kW)	90
FC transient response 10-90% power (s)	1.5

Three different energy storage systems were considered in the simulation. These included two battery storage systems (NiMH and Li-ion) and ultra-capacitors (ultra-cap). The simulation was made using a single energy storage system, represented as 1-ESS or a combination of two energy storage systems or 2-ESS [2,4,5].

COMPONENT SELECTION and SIZING

FUEL CELL HYBRID ARCHITECTURE - In a FCHEV the primary power source, the PEM fuel cell, is assisted by an ESS like a battery or an ultra-capacitor. The present analysis is based on a single or a combination of two energy storage systems. Because of these combinations, the powertrain hybridization ratio (PHR) is defined as the ratio of power provided by the FC (the primary power source) to the power of the energy storage systems. The 2-ESS configuration allows incorporation of a high specific energy and a high specific power ESS system. This allows the controller to select the best form of power assist for a specific situation leading to potential increase in efficiency and overall fuel economy. In order to maximize the overall system efficiency, it was important to select the right PHR. The PEM fuel cell generally exhibits best efficiency at part load operation, as was found in the present work. Hence, it is desired that PHR be selected to maximize operation of the FC at part load and allow ESS to assist power requirements of the vehicle during transients or unsteady power demand. PHR depends on the type of ESS selected for the powertrain. An ESS with lower specific energy leads to a higher PHR ratio while a high specific energy ESS means lower PHR and a downsized FC since the ESS can support the vehicle power requirements to a greater extent. The present analysis considered these attributes of ESS and varied PHR accordingly.

The electric motor for traction should have sufficient power to meet vehicle requirements at all operating conditions. To attain them at good efficiencies, a brushless permanent magnet motor (UQM PowerPhase) was selected with specifications given in Table 4 [6]. The output of the motor in motoring mode and motor efficiency plots were obtained from the motor manufacturer and were used in the simulation.

Table 4: Traction Motor/Generator Specifications

Peak Torque	550 Nm
Peak Motoring Power	100 kW
Cont. Motoring Power	55 kW
Peak Regen Power	100 kW
Cont. Regen Power	85 kW
Max.Speed (RPM)	5000
Weight	86 kg

PEM FUEL STACK SIZE - The fuel cell stack is the main power source for vehicle propulsion. The stack should be able to propel the vehicle on its own for most of the driving demands should the energy storage system be at reduced capacity. The fuel cell stack should be sized so as to maximize the powertrain efficiency by making the best use of the ESS [2,5]. The power output and efficiency of the laboratory PEMFC were scaled to the appropriate stack size used in the vehicle. The stack characteristics, based on laboratory tests, were

incorporated in the simulation with 1ESS or 2ESS energy storage systems. The stack power was varied over a range of 30 kW to 90 kW to assess the impact of the main power source with the default size set at 50 kW.

The PEM Fuel cell stack requires several additional components (balance of plant or BOP) to operate it effectively. The BOP is made up of auxiliary/supporting hardware to maintain and control the fuel cell operation and performance. The major components in the BOP are: compressor, pump, expander and radiator with fan. Each component of the BOP has its own operating efficiency. Selection of inefficient components or operating the component at off-optimum point eventually leads to reduction in vehicle fuel economy.

The PSAT simulation program included default BOP components with efficiencies tailored to the plant operation. In this simulation, the default values of component power and efficiencies were used.

Figure 4. 1-ESS Configuration with PEMFC

ENERGY STORAGE AND STRATEGY – The energy storage in the FCHEV must be able to supply adequate power during transients and steady power demands. It should be sized to absorb energy at adequate rate during regeneration such as braking and deceleration. Some of the functions of the energy storage system in a FCHEV are:

- Fuel cell startup and shut down assist
- Provide tractive power during ESS only mode
- Capture and store regenerative braking energy
- Power assist during high power driving situations like acceleration, gradeability in various drive cycles
- Electrical accessory loads

Table 5: Energy Storage System Comparison

Characteristic	NiMH	Li-Ion	Ultra-Cap
Cell Voltage (V)	1.2	3.6	2.5- 3.0
Sp. Power (kW/kg)	0.7- 1	1.0-1.2	8-10
Sp Energy (kWh/kg)	0.04- .08	.11- .15	0.005- .01

Based on these considerations, three storage systems were included in the simulation: NiMH batteries, Li-Ion batteries and ultra-capacitors [7,8]. Li-Ion has high specific energy while ultra-capacitors exhibit high specific power. The NiMH has lower specific energy and lower specific power but has some cost advantage over

the other two energy storage systems [7,9]. Table 5 shows comparative characteristics of the three energy systems and Table 6 shows capacity of the three systems selected in the simulation

The simulation included each of these storage media individually (1-ESS) or in combination (2-ESS). The 2-ESS configuration, with a battery and ultracaps storage, allowed proper load sharing. The ultracaps are effective during fast transient power demands while the battery storage provided power during steady or slowly increasing demands.

Table 6. Energy Storage System Specifications

Characteristic	NiMH	Li-Ion	Ultracap
Voltage (V)	300	260	62.5
Nom. Capacity(C/3)	28 Ah	6 Ah	2500 F
Energy (kWh)	10	6.5	0.12
Number of Cells	300	75	25
Weight (kg)	87	45	18

The models with 1-ESS and 2-ESS systems used similar control strategies to maximize fuel efficiency of the powertrain, as shown in Figures 4 and 5, respectively. But the ESS assist profiles were different to reflect different operational performance and efficiency characteristics of the individual ESS used in the system. The propulsion motor provided the requested torque at the wheel. The size of the ESS and the FC limit available torque. If the ESS state of charge is low, the ESS is not used to provide energy for propulsion.

Figure 5. 2-ESS Configuration with PEMFC

The controls in PSAT provide three outputs: (a) Motor torque (b) FC on or off and (c) FC power.

The control strategy used in the 1-ESS system is designed to maximize fuel efficiency of the powertrain but with different assist profiles for each individual ESS to reflect its characteristics. The electric motor is used to deliver the requested torque at the vehicle wheels. If the ESS state of charge (SOC) is too low (below the set limit) all the torque is provided by the FC, with no power delivered by the ESS.

The 2-ESS control strategy works in a similar manner as the 1-ESS but the difference lies in the controls of each

ESS. Unlike the 1-ESS, where all the assist is derived from one source, the controller in this case operates in such a way that the first ESS (Li-Ion in this case) provides average power demands while the second ESS (the Ultracaps) provides power during sharp transients. Both ESSs are limited by their maximum charge and discharge characteristics. Both SOC are regulated to avoid complete energy depletion. If the combined 2-ESS is not able to meet the requested power demand then the motor torque is limited.

RESULTS

The FCHEV vehicle configurations with one or two ESS storage system were simulated for the following drive cycles and performance.

- Urban Dynamometer Driving Schedule (UDDS)
- Highway Fuel Economy Test (HWFET)
- Combined drive cycle
- 0 – 60 MPH acceleration Time
- Maximum Vehicle Speed

The stack power for each of the ESS configuration was varied by keeping the ESS size and other vehicle attributes unaltered. The objective of the parametric study was to find the FC stack power, with experimentally derived FC performance characteristics, that would result in best fuel economy and vehicle performance.

Figure 6 shows combined fuel economy (highway and urban combined), in mpg of gasoline equivalent, when a single ESS source was used. The best fuel economy was obtained when the stack power output was 60 to 70 kW in conjunction with Li-Ion battery storage. Li-Ion batteries have high charge and discharge efficiency compared to NiMH batteries. Li-Ion battery storage had about 3% better fuel economy over NiMH and about 7% over ultra-capacitor storage, respectively. Reducing the stack size to below 50 kW resulted in fuel economy penalty of about 3% over the best fuel economy operation.

There is an optimum fuel cell stack power for each of the ESS configuration where the efficiency of the powertrain

is the highest due to maximized usage of the ESS and part load operation of the FC stack. Below this optimum point the fuel efficiency decreases due to increased loading of the balance of plant, which does not decrease in proportion to the fuel cell power downsizing, requiring the stack to operate at high power levels. On the other hand, the fuel economy decreases above the optimum power level due to decreased usage of the ESS power, which is more efficient than fuel cell power. Figure 7 shows fuel economy of the three ESSs when the vehicle was driven on urban dynamometer driving cycle. As expected, a hybrid powertrain provided better fuel economy on urban cycle than highway or combined cycle. Again, the Li-Ion storage has better fuel economy than the other two energy storage systems.

The use of ultra-capacitors as a single energy storage medium produced poor fuel economy of all the three storage systems. Ultra-capacitors have high specific power but low energy storage capability for its size [2,5]. They can provide a quick burst of power for a short period of time, a desired attribute for vehicle acceleration over a short period of time.

Their low energy storage capacity does not lend them as a good energy storage medium compared to NiMH or

the Li-Ion battery storage system. However, when used in conjunction with a high-energy storage device, ultra-capacitors have advantage, as shown in Figure 9. Adding ultra-capacitors to Li-Ion battery system provided improved fuel economy, the best economy being achieved when the stack power output was around 50 kW. The fuel economy improvement of the 2-ESS (Li-Ion and ultracap) was about 9% over the Li-Ion battery storage on combined drive cycle. Similar improvement was realized when ultracaps were combined with NiMH battery storage system, as shown in Figure 9.

Detailed analysis of fuel economy shows that the biggest improvement was in the urban drive cycle where the ultracap ESS recovers higher percentage of regenerative braking energy. Highway cycle, which has less drive cycle variations, provided lower fuel economy gains.

The vehicle acceleration time is dictated by the amount of energy stored, the energy discharge characteristics and the power output of the stack. Figure 9 shows a comparison of acceleration time with 1-ESS storage and varying stack power. FC power below 30 kW resulted in long acceleration time which would not be acceptable to users. NiMH and Li-Ion battery storage are capable of accelerating the vehicle in about 10 seconds, an acceptable time, when the FC power was at least 40 kW. Because of low energy storage capacity of ultra-capacitors this system had long acceleration time and would not be suitable for this application by itself. But combining ultra-capacitors with NiMH or the Li-Ion batteries reduced 0-100 kph acceleration time, as shown in Figure 10. The acceleration time with 30 kW stack power was comparable to the time that is expected of a similar vehicle powered by a spark ignition engine.

COMPARISON OF POWER ASSIST PROFILE

The major differences between 1-ESS and 2-ESS FC based HEV are the operation of the powertrain and the amount of assist provided by the energy storage systems to the FC and vehicle power demands.

A series FCHEV with 2-ESSs has a higher powertrain hybridization ratio and the control strategy maximizes utilization of the stored energy by higher amount of power assist during acceleration and transients and by recovering a greater amount of available regenerative braking energy. Figures 11 and 12 show two distinct profiles of the operational characteristics of the two-powertrain configurations for the same section of the highway fuel economy test drive cycle.

The 1-ESS NiMH battery storage system supplies most of the power during the first 5 seconds of operation on highway drive cycle. Then the stack starts to power almost all of the 40 kW required for propulsion and the BOP operation. In contrast, power sharing is achieved quite effectively in the 2-ESS (NiMH + ultracaps) system. The ultra-capacitors provide most of the power during the very first portion of acceleration, followed by power sharing between ultracaps and FC and then by FC and the batteries. Unlike in 1-ESS system, the Li-Ion

Figure 12. Power Profile with NiMH+ Ultracaps

battery storage in the 2-ESS system does not provide power during the initial phase of vehicle operation. The powertrain control system is responsible for deciding power sharing between the ESS and the PEMFC. When the ESS state of charge is low, power to the motor is supplied by the PEMFC. The controller limits the maximum level of ESS discharge before charging must occur. ESS charging also occurs during regeneration and deceleration. As can be seen in Figure 11, the FC stack operates at almost steady power level for most of the drive cycle time. Such an operation results in improved fuel economy.

The simulation did not include stack dynamics during dynamic operation of the powertrain. The stack dynamics is now being investigated and will be included in future work.

CONCLUSIONS

A fuel cell hybrid electric vehicle was simulated using a model in PSAT. The model utilized experimentally determined PEM fuel cell characteristics with reactant gases at 70 C and 100% relative humidity. The flow rates of gases were at $\lambda = 1.2$ for hydrogen and 2.5 for air, respectively. Batteries and ultra-capacitors were used as energy storage media. The best fuel economy was realized with Li-Ion batteries when single energy storage was used. A combination of Li-Ion batteries and ultra-capacitors resulted in improved fuel economy of about 9% over 1-ESS Li-Ion storage. Ultra-capacitors, by themselves, did not provide good fuel economy compared to battery storage and the vehicle acceleration time was too long. The combination of battery and ultra-capacitor storage allowed efficient power sharing between the three devices, allowing the stack to operate at almost steady conditions over the simulated test cycle. An energy storage system with high

specific energy and high specific power would be better suited to meet the powertrain requirements.

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NOMANCLATURE

A = vehicle frontal area (m^2)
M = vehicle mass (kg)
MC = motor control and accessory power
 P_{road} = vehicle power (kW)
 P_{roll} = power due to rolling resistance (kW)
 P_{hill} = power for climbing (kW)
 P_{aero} = power due to aerodynamic resistance (kW)
 P_{accel} = power required for acceleration (kW)
V = vehicle speed (kph)
 ρ = air density (kg/m^3)