Final Report

Department of Energy Award: DE-FG26-05NT42615

Project Title:
GATE Center for Automotive Fuel Cell Systems at Virginia Tech

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Project performance period: 10/1/2005 – 5/30/2011
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Distribution: Unlimited

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GATE Center for Automotive Fuel Cell Systems at Virginia Tech

Executive Summary

The Virginia Tech GATE Center for Automotive Fuel Cell Systems (CAFCS) achieved the following objectives in support of the domestic automotive industry:

- Expanded and updated fuel cell and vehicle technologies education programs;
- Conducted industry directed research in three thrust areas – development and characterization of materials for PEM fuel cells; performance and durability modeling for PEM fuel cells; and fuel cell systems design and optimization, including hybrid and plug-in hybrid fuel cell vehicles;
- Developed MS and Ph.D. engineers and scientists who are pursuing careers related to fuel cells and automotive applications;
- Published research results that provide industry with new knowledge which contributes to the advancement of fuel cell and vehicle systems commercialization.

With support from the Dept. of Energy, the CAFCS upgraded existing graduate course offerings; introduced a hands-on laboratory component that make use of Virginia Tech's comprehensive laboratory facilities, funded 15 GATE Fellowships over a five year period; and expanded our program of industry interaction to improve student awareness of challenges and opportunities in the automotive industry. GATE Center graduate students have a state-of-the-art research experience preparing them for a career to contribute to the advancement fuel cell and vehicle technologies.

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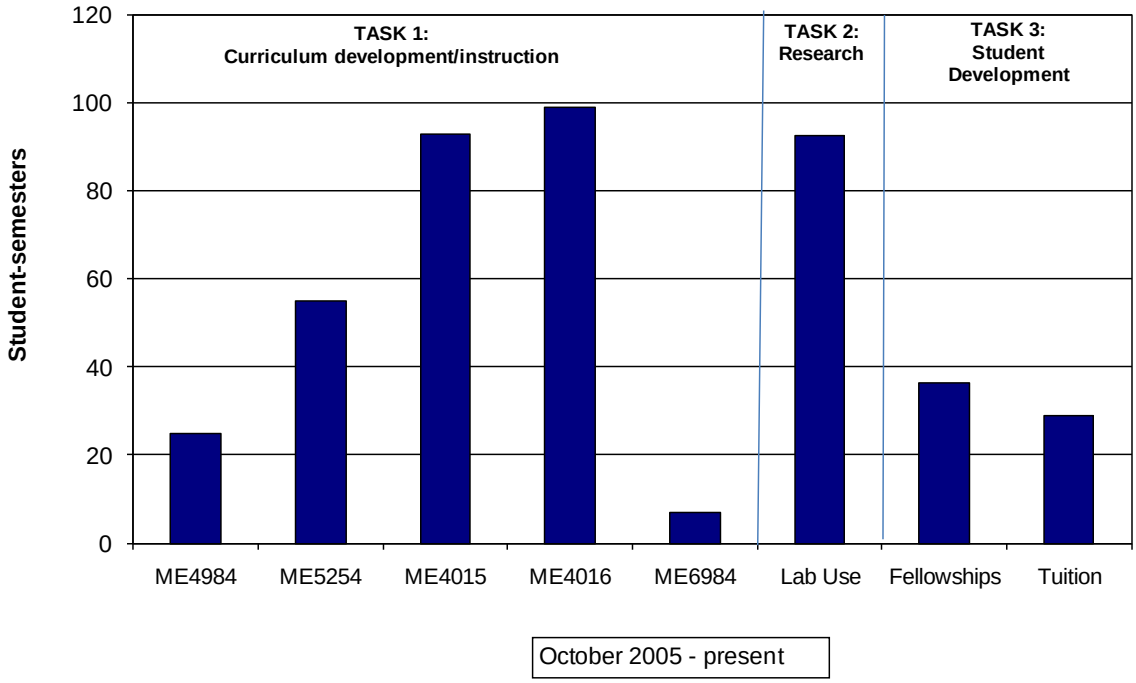
Project Summary

The goals and objectives of the project were accomplished and results from the first 3 tasks are summarized in the following figure.



The forth task, Dissemination, was accomplished by many publications and conference presentations, and are included in the following detailed results from the project. None of the publications were directly or exclusively funded by the project, and are thus not considered a product of the award.

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DE-FG26-05NT42615

Progress Summary
Year Five 10/1/2009 – 9/30/2010
October 29, 2010

I. TASK 1 – CURRICULUM DEVELOPMENT

A. Taught ME 4015/4016: Engineering Design and Project, Fall 2009 and Spring 2010 to 24 Mechanical Engineering seniors, for Advanced Vehicle Technology Competition which included development of a plug-in hybrid electric vehicle. This effort is continuing for ME 4015/4016 for Fall 2010 and Spring 2011 with 24 students.

B. Taught ME 4554 Advanced Technology Vehicles to 42 advanced undergraduate and graduate students in Fall 2009, where we covered performance and fuel economy modeling of electric, plug-in hybrid electric and fuel cell hybrid vehicles. This effort is continuing for ME 4554 for Fall 2010 with 44 students.

C. Prepared for ME 5254: Fuel Cell Systems and taught to 15 advanced undergraduate and graduate students in Spring 2010. A laboratory module was improved for the course. In this exercise, students assemble a fuel cell, evaluate performance by measuring a polarization curve and isolate individual losses using electrochemical impedance spectroscopy.

D. Developed ME6984: Experimental and Analytical Techniques for PEM Fuel Cells and taught to 7 graduate students in Fall 2010. In this new course students develop a basic understanding of the fundamental concepts of thermodynamics, transport processes, and electrochemistry as they relate to fuel cells. They study how these phenomena can be observed and measured and how fuel cell components can be characterized. Techniques include measurement of polarization curves, electrochemical impedance spectroscopy, linear sweep voltammetry, cyclic voltammetry, BET surface area analysis, mesopore characterization, and gas diffusion layer characterization. Students apply their new knowledge to critically examine current issues in fuel cell research.

II. TASK 2 – RESEARCH

A. Development and characterization of materials for PEM fuel cells

Engaged in research in the following areas related to material characterization:

- Development of a non-linear viscoelastic model for stress prediction in membranes comprised of PFCB/PVDF blends. *(Jessica Wright)*
- Characterization of the fracture energy of PFCB/PVDF membranes using a knife slit test. *(Ashley Gordon))*
- Evaluation of the biaxial strength of PFSA membranes using pressure loaded blister tests. *(Affiliated project[1])*

[1] Affiliated projects are team-based projects that involve GATE funded students and faculty but for which funding for the specific task is from a source other than the GATE Center.

- Development of a life prediction model for fuel cell membranes. *(Affiliated project)*
- Development of characterization techniques for capillary pressure-saturation curves for materials of mixed wetability (i.e. GDLs). (Andrew Van Dyke)

B. Numerical modeling of fuel cell phenomena

Engaged in research in the following areas related to modeling of PEM fuel cells:

- Development and application of atomistic-level models using quantum thermodynamics for the non-equilibrium process description of hydrogen storage on carbon nanotubes (Charles Smith)
- Development of models for the mesoscopic (i.e., microscopic-level) modeling of reacting mixture flows with contaminants (e.g, CrO3) in the micro-structures of SOFC cathode electrodelayers using kinetic theory (Gayle Kestell) *(Affiliated project).*
- Modeling, development, and testing of hydrogen and methanol micro-tubular fuel cells and stacks for use as power plants in microair vehicles (Matthew Miller and David Woolard) *(Affiliated project).*

C. Fuel cell systems synthesis/design and control/operation optimization

Engaged in research in the following areas related to system design and optimization:

- Development of transient thermodynamic, geometric, kinetic, cost, and control component and system performance models and the application of decomposition strategies to the large-scale single and multi-objective optimization under uncertainty of the synthesis/design and operation/control of a natural gas based 5 kWe PEMFC system consisting of three subsystems: fuel processing, work recovery/air supply, and fuel cell stack (Meng Wang and Kihyung Kim) *(Affiliated project).*
- Development of first and second law based simulation models in AspenPlus^{TM} in order to do detailed exergy analyses of the performance and degradation of hybrid SOFC/GT/ST cycles (Martin Lustfeld and Sergio Cano) (*Affiliated project).*
- Modeling and simulation study of regenerative fuel cell based renewable energy storage (Matteo M. Coppola and Sergio Cano) (*Affiliated project).*

D. Fuel Cell and Hybrid Electric Vehicle energy use and environmental impact

- Impact of drive cycle and temperature on electric drive vehicle efficiency (Mark Meyer)
- Accessory loads in electric drive vehicles (Donald Perkins)
- Plug-in hybrid vehicles using grid electricity and E85 fuels

E. Student progress on research projects

- Andrew Van Dyke: continuing MS on "Evaluation of water transport parameters of commercial gas diffusion media," May 2011.
- Jessica Wright: continuing MS on "Development of a Non-Linear Stress Model for PFCB/PVDF Polymer Electrolytes," May 2011.
- Ashley Gordon: continuing MS on "Alternative Materials and Fuels for Low Temperature Fuel Cells," May 2012.

- Charles Smith: continuing PhD on "Development and application of quantum thermodynamics to the atomistic-level modeling of non-equilibrium phenomena (e.g., hydrogen storage on carbon nanotubes)," August 2011.
- Gayle Kestell, completed MS thesis on "Model of chromium poisoning in the cathode of a solid oxide fuel cell using the lattice Boltzmann method," February 2010 (*Affiliated project*).
- Michael Diaz, began PhD program on "Control System Stability in Hybrid Electric Vehicles", left program summer 2010 to work at GM.
- Donald Perkins, began MS on "Accessory loads in electric drive vehicles", May 2011.
- Mark Meyer, continuing joint VT/TUD MS on "Impact of Five Cycle Fuel Economy Testing on Electric Drive Vehicles", Dec, 2011.

III. TASK 3 - STUDENT RECRUITMENT AND GATE FELLOWS SUPPORT

- Provided support for GATE fellows, Charles Smith, started Spring 2007, Michael Diaz, and Mark Meyer, started Fall 2010, with research topics as outlined in the previous section.
- Provided support for Donald Perkins who is working toward his MS on accessory loads in electric drive vehicles, expected to graduate 2011.
- Provided support for Andrew van Dyke who is working toward his MS on water transport properties of diffusion media, expected to graduate 2011.

IV. TASK 4 - DISSEMINATION

A. Publications:

1. Kim, K., von Spakovsky, M. R., Wang, M., Nelson, D., 2010, "A Hybrid Multi-level Optimization Approach for the Dynamic Synthesis/Design and Operation/Control under Uncertainty of a Fuel Cell System," *Energy: The International Journal*, doi:10.1016/j.energy.2010.08.024.
2. Smith, C. E., Sciacovelli, A., von Spakovsky, M. R., Verda, V., 2010, "3D Quantum Thermodynamic Description of the Non-equilibrium Behavior of an Unbounded System at an Atomistic Level," *Journal of Physics: Conference Series*, 237, 012022, presented at the Symmetries of Science Symposium XIV, Institute of Physics (IOP), Bregenz, Austria, July 19-24.
3. Sciacovelli, A., Smith, C. E., Verda, V., von Spakovsky, M. R., 2010, "Quantum Thermodynamics: Non-equilibrium 3D Description of an Unbounded System at an Atomistic Level," *The International Journal of Thermodynamics*, vol. 13 (no. 1), pp. 23-33.
4. Cano-Andrade, S., Hernandez-Guerrero, A. and von Spakovsky, M. R., 2010, "Current Density Curves for Radial Configuration PEMFCs," *Energy: The International Journal*, available on-line at http://dx.doi.org/10.1016/j.energy.2009.07.045, 35(2) (February 2010) 920–927.
5. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2010, "Uncertainty Analysis with Multi-objective Optimization for the Synthesis/Design and Operation/Control of a

PEMFC Fuel Processing Subsystem," ASME, *Journal of Fuel Cell Science and Technology*, in preparation.

6. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2010, "Dynamic Optimization under Uncertainty of the Synthesis/Design and Operation/Control of a PEMFC System," ASME, *Journal of Power Sources*, in preparation.
7. Kestell, G., von Spakovsky, M.R., Asinari, P., 2010, "Modeling Cr Poisoning in a SOFC Cathode using the Lattice Boltzmann Method," *Journal of Power Sources*, in preparation.
8. Beretta, G.-P., von Spakovsky, M. R., 2010, "Quantum thermodynamic framework for describing the non-equilibrium behavior of a chemically reactive system at an atomistic level," *Journal of Chemical Physics*, in preparation
9. Frank Falcone, Douglas Nelson, James Burns (2010), "Closed Loop Transaxle Synchronization Control Design", SAE paper 2010-01-0817 in Engine Control and Optimization in Hybrid Powertrains SP-2284 presented *at SAE 2010 World Congress & Exhibition*, April 13-15, 2010, Detroit, MI; 20 pages.
10. Michael Wahlstrom, Frank Falcone, and Douglas Nelson (2010), "Integrating Hardware-in-the-Loop into University Automotive Engineering Programs Using Advanced Vehicle Technology Competitions", paper AC 2010-1409, *American Society for Engineering Education 117th Annual Conference & Exposition*, June 20 - 23, 2010, Louisville, Kentucky, 10 pages.
11. Lynn R. Gantt, Patrick M. Walsh, and Douglas J. Nelson (2010), "DESIGN AND DEVELOPMENT PROCESS FOR A RANGE EXTENDED SPLIT PARALLEL HYBRID ELECTRIC VEHICLE", Paper DETC2010-28576 accepted for publication in the Proceedings of the *ASME 2010 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference IDETC/CIE 2010* August 15-18, 2010, Montreal, Quebec, Canada, 14 pages.
12. Grohs, J.R., Y.Q. Li, D.A. Dillard, S.W. Case, M.W. Ellis, Y.H. Lai, and C.S. Gittleman, "Evaluating the time and temperature dependent biaxial strength of Gore-Select (R) series 57 proton exchange membrane using a pressure loaded blister test," *Journal of Power Sources*, 195(2): p. 527-531, 2010.
13. Patankar, K., D.A. Dillard, S.W. Case, M.W. Ellis, Y.Q. Li, Y.H. Lai, M.K. Budinski, and C.S. Gittleman, "Characterizing Fracture Energy of Proton Exchange Membranes Using a Knife Slit Test," *Journal of Polymer Science Part B-Polymer Physics*, 48(3): p. 333-343, 2010.

Other papers are in process for each of our research projects.

B. Professional Meetings:

1. Michael Ellis was chair of a session on "Fuel Cell Materials: Bipolar Plate and Other Stack Materials" at the *8th International Conference on Fuel Cell Science, Engineering and Technology* held in New York, NY June 2010.
2. Michael Ellis gave an invited talk titled, "Evaluation of Water Transport Characteristics of PEM Fuel Cell Diffusion Media" at Michigan Tech, Houghton, MI on September 30, 2010.

3. Michael von Spakovsky was chairman of a session on the optimization of energy systems, *Advanced Energy Systems Division*, ASME International Mechanical Engineering Congress and Exposition, Boston, MA, Oct. - November 2008.
4. Michael von Spakovsky, short course, *Generalization of Thermodynamics to Microscopic Systems: Equilibrium and Non-Equilibrium Considerations*, Summer School of Thermodynamics, University of Roma "La Sapienza", June 21 - July 3, 2010.
5. Michael von Spakovsky, chairman of a session on the fundamentals of thermodynamics at the International Conference on Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'10), Lausanne, Switzerland, ASME, June 14-17, 2010.
6. Michael von Spakovsky, invited seminar speaker, *A Hybrid Multi-level Optimization Approach for the Dynamic Synthesis/Design and Operation/Control under Uncertainty of a Fuel Cell System*, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, August 26, 2010.
7. Michael von Spakovsky, invited seminar speaker, *Generalization of Thermodynamics to Microscopic Systems: Equilibrium and Non-equilibrium Considerations – Applications*, University of Brescia, Brescia, Italy, July 19, 2010.
8. Michael von Spakovsky, invited seminar speaker, *Generalization of Thermodynamics to Microscopic Systems: Equilibrium and Non-equilibrium Considerations*, University of Brescia, Brescia, Italy, July 12, 2010.
9. Michael von Spakovsky, invited seminar speaker, *Generalization of Thermodynamics to the Microscopic Scale: Equilibrium and Non-Equilibrium, Efficiency*, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'10), keynote address, *Lausanne, Switzerland, ASME, June 14-17.*

V. TASK 5 - INDUSTRY INTERACTION

A. *Faculty and* student attendance at industry forums:
   - Faculty and students from the Virginia Tech GATE Center attended many events during the period including 2010 EcoCAR Challenge; 2010 Challenge Bibendum in Rio De Janeiro, Brazil, 2010 SAE Congress, Detroit, MI; 2010 8th International Fuel Cell Science; Engineering and Technology Conference, New York, NY. The Virginia Tech GATE Center also hosted visits from many industry representatives during the past year.

B. Research project collaboration with automotive companies
   - Michael Ellis, Jessica Wright, and Ashley Gordon (graduate researchers) participated in bi-weekly web-meetings with other VT researchers and GM researchers working on PEM membrane research.

C. Research project presentations to government organizations
   - Doug Nelson attended the DoE Merit Review meeting on 8-10 June 2010.
   - Michael von Spakovsky, presentation of proposed research activities on *Non-equilibrium Material Transport and Interaction Study in Extreme Environments – Experiment and Modeling* and on *Stochastic Multilevel Dynamic Optimization for Uncertain Process Systems* to DOE NETL personnel, Pittsburgh, PA, February 8, 2010.
   - Michael von Spakovsky, presentation of proposed research activities on *Material Interactions in Extreme Environments – Experiment and Modeling* and on *Stochastic Multi-level/Multi-objective Dynamic Modeling and Optimization for*

Uncertain Process Systems to DOE NETL personnel visiting Virginia Tech, Blacksburg, VA, April 22, 2010.

- Michael von Spakovsky, poster presentation on *Non-equilibrium Material Transport and Interaction Studies in Extreme Environments – Experiment and Modeling* and on *Stochastic Multi-level/Multi-objective Optimization of Uncertain Process Systems* to DOE NETL personnel, Pittsburgh, PA, May 3-4, 2010.

D. Campus Visits by Industry
   - Dr. Yeh-Hung Lai, General Motors Fuel Cell Research
     - Research collaboration
     - Research Presentation: Viscoelestic Framework for Durability of PEM Materials
   - Mr. Charles Strickler, Ecolectrix, LLC
     - Research collaboration
   - Mr. Jonas Gunter, Luna Innovations, Inc.
     - Research on materials development for micro-tubular fuel cells for micro-air vehicles
   - Dr. Yongquiang Li, GM
     - Research collaboration

E. Graduate Students hired in fuel cell and/or automotive field[2]
   - Michael Diaz, GM hybrid controls 2010. (left Ph.D. program in 2010)
   - Andrew van Dyke (M.S. continuing): BASF Fuel Cells, June 2010

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Center for Automotive Fuel Cell Systems
http://www.me.vt.edu/people/faculty/nelson.html

Faculty Advisor, Hybrid Electric Vehicle Team of VA Tech
http://www.me.vt.edu/hevt

[2] Includes students supported directly by GATE and students working on GATE affiliated projects

GATE Center for Automotive Fuel Cell Systems at Virginia Tech

DE-FG26-05NT42615

Progress Summary
Year Four 10/1/2008 – 9/30/2009
October 30, 2009

I. TASK 1 – CURRICULUM DEVELOPMENT

A. Taught ME 4015/4016: Engineering Design and Project, Fall 2008 and Spring 2009 to 17 Mechanical Engineering seniors, for Advanced Vehicle Technology Competition which included development of a demonstration hydrogen fuel cell APU module. This effort is continuing for ME 4015/4016 for Fall 2009 and Spring 2010 with 24 students.

B. Taught ME 4554 Advanced Technology Vehicles to 46 advanced undergraduate and graduate students in Fall 2008, where we covered performance and fuel economy modeling of electric, plug-in hybrid electric and fuel cell hybrid vehicles. This effort is continuing for ME 4554 for Fall 2009 with 42 students.

C. Prepared for ME 5254: Fuel Cell Systems and taught to 11 advanced undergraduate and graduate students in Spring 2009. A laboratory module was improved for the course. In this exercise, students assemble a fuel cell, evaluate performance by measuring a polarization curve and isolate individual losses using electrochemical impedance spectroscopy.

II. TASK 2 – RESEARCH

A. Development and characterization of materials for PEM fuel cells

Engaged in research in the following areas related to material characterization:

- Development of experimental and analytical tools to assess susceptibility to shorting by penetration. (Chris Fox)
- Development of a constitutive model for PFSA viscoelastic properties. *(Affiliated project[1])*
- Characterization of the fracture energy of PFSA membranes using a knife slit test. *(Affiliated project)*
- Evaluation of the biaxial strength of PFSA membranes using pressure loaded blister tests. *(Affiliated project)*
- Development of a life prediction model for fuel cell membranes. *(Affiliated project)*
- Development of characterization techniques for capillary pressure-saturation curves for materials of mixed wetability (i.e. GDLs). (Andrew Van Dyke)
- Development of characterization techniques for relative permeability in gas diffusion media. (Andrew Van Dyke, Wesley Southall-UG researcher)

[1] Affiliated projects are team-based projects that involve GATE funded students and faculty but for which funding for the specific task is from a source other than the GATE Center.

B. Performance and durability modeling of PEM fuel cells

Engaged in research in the following areas related to modeling of PEM fuel cells:

- Development and application of atomistic-level models using quantum thermodynamics for the non-equilibrium process description of hydrogen storage on carbon nanotubes (Charles Smith)
- Development of models for the mesoscopic (i.e., microscopic-level) modeling of reacting mixture flows with contaminants (e.g, CrO3) in the micro-structures of SOFC cathode electrodelayers using kinetic theory (Gayle Kestell) *(Affiliated project).*
- Modeling, development, and testing of hydrogen and methanol micro-tubular fuel cells and stacks for use as power plants in microair vehicles (Matthew Miller and David Woolard) *(Affiliated project).*

C. Fuel cell systems synthesis/design and control/operation optimization

Engaged in research in the following areas related to system design and optimization:

- Development of transient thermodynamic, geometric, kinetic, cost, and control component and system performance models and the application of decomposition strategies to the large-scale single and multi-objective optimization under uncertainty of the synthesis/design and operation/control of a natural gas based 5 kWe PEMFC system consisting of three subsystems: fuel processing, work recovery/air supply, and fuel cell stack (Meng Wang and Kihyung Kim) *(Affiliated project).*
- Development of first and second law based simulation models in AspenPlus^{TM} in order to do detailed exergy analyses of the performance and degradation of hybrid SOFC/GT/ST cycles (Martin Lustfeld and Sergio Cano) (*Affiliated project).*

D. Fuel Cell and Hybrid Electric Vehicle energy use and environmental impact

- Analysis of the environmental characteristics of an advanced technology/alternative fueled vehicle fleet including hydrogen and fuel cell vehicles (Jeongwoo Lee) *(Affiliated project)*
- Vehicle Inertia Impact on Fuel Consumption using Pulse and Glide (Acceleration and Coast) Driving Strategy (Jeongwoo Lee)
- Plug-in hybrid vehicles using grid electricity, hydrogen and E85 fuels

E. Student progress on research projects

- Andrew Van Dyke: continuing MS on “Evaluation of water transport parameters of commercial gas diffusion media,” May 2010.
- Charles Smith: continuing PhD on “Development and application of quantum thermodynamics to the atomistic-level modeling of non-equilibrium phenomena (e.g., hydrogen storage on carbon nanotubes),” May 2011.
- Jeongwoo Lee: completed PhD dissertation on “Vehicle Inertia Impact on Fuel Consumption”, September, 2009.

III. TASK 3 - STUDENT RECRUITMENT AND GATE FELLOWS SUPPORT

- Provided support for GATE fellows, Charles Smith, started Spring 2007, and Jeongwoo Lee, started Jan 2007, with research topics as outlined in the previous section.
- Provided support for Andrew van Dyke who is working toward his MS on water transport properties of diffusion media, expected to graduate 2010.

IV. TASK 4 - DISSEMINATION

A. Publications:

1. Cano-Andrade, S., Hernandez-Guerrero, A. and von Spakovsky, M. R., 2009, "Current Density Curves for Radial Configuration PEMFCs," *Energy: The International Journal*, available on-line at http://dx.doi.org/10.1016/j.energy.2009.07.045, in press.
2. Arsalis, A., Calise, F., von Spakovsky, M.R., 2009, "Thermoeconomic Modeling and Parametric Study of Hybrid Solid Oxide Fuel Cell – Gas Turbine – Steam Turbine Power Plants Ranging from 1.5 MWe to 10 MWe," *Journal of Fuel Cell Science and Technology*, ASME, N.Y., N.Y., vol. 6, issue 1, 011015 (12 pages), February.
3. Verda, V., von Spakovsky, M.R., 2008, "2D Detailed Planar SOFC CFD Model for Predicting the Effects of Cell Performance Degradation," *Journal of Fuel Cell Science and Technology*, ASME, N.Y., N.Y., vol. 6, issue 1, 011005 (9 pages), February.
4. Sciacovelli, A., Smith, C. E., Verda, V., von Spakovsky, M. R., 2009, "3D Quantum Thermodynamic Description of the Non-equilibrium Behavior of an Unbounded System at an Atomistic Level," *Journal of Physics Conference Series*, Symmetries of Science Symposium XIV, Institute of Physics (IOP), Bregenz, Austria, July 19-24, in preparation.
5. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2009, "Uncertainty Analysis with Multi-objective Optimization for the Synthesis/Design and Operation/Control of a PEMFC Fuel Processing Subsystem," ASME, *Journal of Fuel Cell Science and Technology*, in preparation.
6. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2009, "Dynamic Optimization under Uncertainty of the Synthesis/Design and Operation/Control of a PEMFC System," ASME, *Journal of Fuel Cell Science and Technology*, in preparation.
7. J. D. Sole, M.W. Ellis, D.A. Dillard, "Experimental and analytical study of gas diffusion layer materials for ribbon fuel cells," *ASME Journal of Fuel Cell Science and Technology*, Vol 6 (4), pp. 041010-1 – 041010-7.
8. Sciacovelli, A., Smith, C. E., Verda, V., von Spakovsky, M. R., 2009, "Quantum Thermodynamics: Non-equilibrium 3D Description of an Unbounded System at an Atomistic Level," *Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'09)*, Parana, Brazil, ASME, Aug. 31 – Sept. 3.
9. Kim, K., von Spakovsky, M. R., Wang, M., 2009, "Application of a Hybrid Multi-level Optimization Approach to the Dynamic Synthesis/Design and Operation/Control under Uncertainty of a PEMFC System," *Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'09)*, Parana, Brazil, ASME, Aug. 31 – Sept. 3.

10. M. Pestrak, Y.Q. Li, S.W. Case, David A. Dillard, Michael W. Ellis,Yeh-Hung Lai, Craig S. Gittleman, “The Effect of Catalyst Layer Cracks on the Fatigue Lifetimes of MEA,” *7th International Conference on Fuel Cell Science, Engineering, and Technology*, 2009.
11. J.D. Sole and M.W. Ellis, “Development of a Method for Determining the Two-Phase Relative Permeability Relationships in the Gas Diffusion Layers of PEM Fuel Cells”, *7th International Conference on Fuel Cell Science, Engineering, and Technology*, 2009.
12. Stover, Michael, Lynn Gantt, Graham Burkholder, Adam Robinson, and Douglas J. Nelson (2009), ″Design and Development Process for a Plug-in E85 Split Parallel Architecture Hybrid Electric Vehicle″, Paper 2460156 accepted for publication at EVS-24, *The 24th International Battery, Hybrid and Fuel Cell Electric Vehicle Symposium and Exhibition*, Stavanger, Norway, May 13-16, 2009.
13. Jeongwoo Lee; Douglas J. Nelson, and Henning Lohse-Busch (2009), ″Vehicle Inertia Impact on Fuel Consumption of Conventional and Hybrid Electric Vehicles Using Acceleration and Coast Driving Strategy″, SAE Paper 2009-01-1322, to be published at *SAE International World Congress*, April 20-23, 2009, Detroit, Mi., 11 pgs.
14. Nelson, Douglas J. and Kurt Johnson, 2009, "Motor and Battery Power Requirements for Plug-In HEVs", Presented at *SAE 2009 Hybrid Vehicle Technologies Symposium*, 12 February 2009, San Diego, California, USA, Published on-line by SAE.
15. von Spakovsky, M.R., Wang, M., Kim, K., and Nelson, D. J., 2009, “Optimal-Control Strategies Based on Comprehensive Modeling and System-Interaction Analysis for Energy-Efficient and Reduced-Emission Fuel-Cell-Energy-Conversion Technologies for Hybrid Stationary and Non-Stationary Applications: Fuel Processing Subsystem (FPS), Fuel Cell Stack Subsystem (SS), and Work Recovery and Air Supply Subsystem (WRAS),” final report, U.S. EPA, EPA Agreement number: RD-83151401-0, January.
16. von Spakovsky, M.R., Smith, C. E., Verda, V., 2008, “Quantum Thermodynamics for the Modeling of Hydrogen Storage on a Carbon Nanotube,” *International Mechanical Engineering Congress and Exposition – IMECE’2008*, ASME Paper No. IMECE2008-67424, N.Y., N.Y., Oct.-Nov.
17. Wang, M., Kim, K., von Spakovsky, M. R., Nelson, D. J., 2008, Multi- versus Single-Level Dynamic Synthesis/Design and Operation/Control Optimizations of a PEMFC System, *International Mechanical Engineering Congress and Exposition* – IMECE’2008, ASME Paper No. IMECE2008-68073, N.Y., N.Y., Oct.-Nov..
18. Wang, M., Kim, K., von Spakovsky, M. R., Nelson, D. J., 2008, Use of State Space in the Dynamic Synthesis/Design and Operation/Control Optimization of a PEMFC System, *International Mechanical Engineering Congress and Exposition* – IMECE’2008, ASME Paper No. IMECE2008-68076, N.Y., N.Y., Oct.-Nov.
19. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2008, Dynamic Synthesis/Design and Operation/Control Optimization under Uncertainty of a PEMFC System, *International Mechanical Engineering Congress and Exposition* – IMECE’2008, ASME Paper No. IMECE2008-68070, N.Y., N.Y., Oct.-Nov.
20. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2008, “Stochastic Modeling and Uncertainty Analysis with Multi-objective Optimization Strategies for the Synthesis/Design and Operation/Control of a PEMFC Fuel Processing Subsystem,” *International Mechanical Engineering Congress and Exposition – IMECE’2008*, ASME Paper No. IMECE2008-68065, N.Y., N.Y., Oct.-Nov.

21. Smith, C. E., Verda, V., von Spakovsky, M. R., 2008, "Quantum Thermodynamics for the Modeling of Non-equilibrium Phenomena," *Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'08)*, keynote address, Cracow, Poland, ASME, June 24-27.
22. Cano-Andrade, S., Hernandez-Guerrero, A. and von Spakovsky, M. R., 2008, "Current Density Curves for Radial Configuration PEMFCs," *Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'08)*, Cracow, Poland, ASME, June 24-27.
23. Li, Y., Grohs, J., Pestrak, M. T., Dillard, D. A., Case, S. W., Ellis, M. W., Lai, Y. H., Gittleman, C. S., and Miller, D. P., "Fatigue and Creep to Leaking Tests of Proton Exchange Membrane Using Pressure-Loaded Blisters", J. Power Sources, Vo. 194, pp. 873-879, 2009.
24. Dillard, D. A., Li, Y., Grohs, J., Case, S. W., Ellis, M. W., Lai, Y. H., Budinski, M. K., and Gittleman, C. S., "On the Use of Pressure-Loaded Blister Tests to Characterize the Strength and Durability of Proton Exchange Membranes". Journal of Fuel Cell Science and Technology, Vol 6 (3), pp. 031014-1 – 031014-8, 2009.
25. Patankar, K., Dillard, D. A., Case, S. W., Ellis, M. W., Lai, Y. H., Budinski, M. K., and Gittleman, C. S., "Hygrothermal Characterization of the Viscoelastic Properties of Gore® Select 57 Proton Exchange Membrane", Mechanics of Time-Dependent Materials, Vol 12 (3), pp. 221-236, 2008.
26. Li, Y., Quincy, J. K., Case, S. W., Ellis, M. W., Dillard, D. A., Lai, Y. H., and Budinski, M. K., "Characterizing the Fracture Resistance of Proton Exchange Membranes". J. Power Sources, Vol 185 (1), pp. 374-380, 2008.
27. Kim, K., Wang, M., von Spakovsky, M. R., Nelson, D. J., 2008, Stochastic Modeling and Uncertainty Analysis with Multi-objective Optimization Strategies for the Synthesis/Design and Operation/ Control of a PEMFC Fuel Processing Subsystem, *International Mechanical Engineering Congress and Exposition* – IMECE'2008, ASME Paper No. IMECE2008-68065, N.Y., N.Y., Oct.-Nov.
28. Mazumder, S.K., Pradhan, S, Hartvigsen, J., Rancruel, D., von Spakovsky, M.R., Kahleel, M., 2008, "A Multidiscipline and Multi-rate Modeling Framework for Planar Solid-oxide-fuel-cell based Power-Conditioning System for Vehicular APU", *Transactions of the Society for Modeling and Simulation*, SMS, September, in press.

Other papers are in process for each of our research projects.

B. Professional Meetings:

1. Michael Ellis was the Track Chair of the Energy Track at *ASME IMECE 2008*, Boston, MA, November 2008.
2. Michael Ellis is chair of the *7th International Conference on Fuel Cell Science, Engineering and Technology* held in Newport Beach, CA June 2009.
3. Michael von Spakovsky was chairman of a session on the optimization of energy systems, *Advanced Energy Systems Division*, ASME International Mechanical Engineering Congress and Exposition, Boston, MA, Oct. - November 2008.

4. Michael von Spakovsky, chair of a session on exergy analysis at the International Conference on Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'08), Krakow, Poland, ASME, June 23-26.
5. Michael von Spakovsky, *3D Quantum Thermodynamic Description of the Non-equilibrium Behavior of an Unbounded System at an Atomistic Level*, Symmetries in Science Conference, Bregenz, Austria, July 23.
6. Michael von Spakovsky, *A General Framework for Modeling Non-Equilibrium Phenomena At Very Small Scales*, TM-STT Thermal Workshop, Propulsion Directorate, AFRL, WPAFB, Ohio, June 10, 2009.
7. Michael von Spakovsky, *Quantum Thermodynamics for the Modeling of Non-equilibrium Phenomena*, Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'08), keynote address, Cracow, Poland, ASME, June 24-27.

V. TASK 5 - INDUSTRY INTERACTION

A. Faculty and student attendance at industry forums:
   - Faculty and students from the Virginia Tech GATE Center attended many events during the period including 2009 EcoCAR Challenge; 2009 EVS-24, Stavanger, Norway, 2009 SAE Congress, Detroit, MI; 2008 6th International Fuel Cell Science; Engineering and Technology Conference, Denver, CO. The Virginia Tech GATE Center also hosted visits from many automotive industry representatives during the past year.

B. Research project collaboration with automotive companies
   - Michael Ellis and Jessica Wright (graduate researcher) participated in bi-weekly web-meetings with other VT researchers and GM researchers working on PEM membrane research.

C. Research project presentations to government organizations

   Doug Nelson attended and presented at the DoE Merit Review meeting on 19 May 2009.

   Michael von Spakovsky, *3D Quantum Thermodynamic Description of the Non-equilibrium Behavior of an Unbounded System at an Atomistic Level*, Air Vehicle Directorate, AFRL, WPAFB, Ohio, August 4, 2009.

   Michael von Spakovsky, *On Modeling Non-Equilibrium Phenomena with Quantum Thermodynamics*, AFRL, WPAFB, Ohio, August 7, 2008.

   Campus Visits by Industry
   - Dr. Yeh-Hung Lai, General Motors Fuel Cell Research
     - Research collaboration
     - Seminars for REU students: Overviews of PEM Durability
     - Research Presentation: Viscoelestic Framework for Durability of PEM Materials
   - Mr. Charles Strickler, Ecolectrix, LLC
     - Research collaboration
   - Mr. Conal Deedy, Volvo Technology of America and Powercell Sv AB
     - Research proposal collaboration
   - Mr. Jonas Gunter, Luna Innovations, Inc.

        - Research on materials development for micro-tubular fuel cells for micro-air vehicles
    - Dr. Yongquiang Li, GM
        - Research collaboration

D. Graduate Students hired in fuel cell and/or automotive field[2]
    - Lohse-Busch, Henning (Ph.D.): ANL 2004, (finished Ph.D. in 2009)

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http://www.me.vt.edu/people/faculty/nelson.html

Faculty Advisor, Hybrid Electric Vehicle Team of VA Tech
http://www.me.vt.edu/hevt

[2] Includes students supported directly by GATE and students working on GATE affiliated projects

GATE Center for Automotive Fuel Cell Systems at Virginia Tech

DE-FG26-05NT42615

Progress Summary
Year Three 10/1/2007 – 9/30/2008
October 31, 2008

I. TASK 1 – CURRICULUM DEVELOPMENT

A. Taught ME 4015/4016: Engineering Design and Project, Fall 2007 and Spring 2008 to 22 Mechanical Engineering seniors, for Advanced Vehicle Technology Competition which included development of a demonstration hydrogen fuel cell APU module. This effort is continuing for ME 4015/4016 for Fall 2008 and Spring 2009 with 17 students.

B. Taught ME 4554 Advanced Technology Vehicles to 46 advanced undergraduate and graduate students in Fall 2007, where we covered performance and fuel economy modeling of electric, plug-in hybrid electric and fuel cell hybrid vehicles. This effort is continuing for ME 4554 for Fall 2008 with 44students.

C. Prepared for ME 5254: Fuel Cell Systems and taught to 13 advanced undergraduate and graduate students in Spring 2008. A new laboratory module was added to the course. In this exercise, students assemble a fuel cell, evaluate performance by measuring a polarization curve and isolate individual losses using electrochemical impedance spectroscopy.

D. Taught ME4015/4016: Engineering Design and Project, Fall 2007 and Spring 2008, to 9 Mechanical Engineering seniors, which included the design, construction, and testing of a passive (with and without wicking) direct methanol fuel cell (DMFC) test fixture for testing 5 cm^2 membrane electrode assemblies (MEAs) based on Nafion™ or BPSH™.

II. TASK 2 – RESEARCH

A. Development and characterization of materials for PEM fuel cells

Engaged in research in the following areas related to material characterization:

- Development of experimental and analytical tools to assess susceptibility to shorting by penetration. (Chris Fox)
- Development of a constitutive model for PFSA viscoelastic properties. *(Affiliated project[1])*
- Characterization of the fracture energy of PFSA membranes using a knife slit test. *(Affiliated project)*
- Evaluation of the biaxial strength of PFSA membranes using pressure loaded blister tests. *(Affiliated project)*
- Development of characterization techniques for capillary pressure-saturation curves for materials of mixed wetability (i.e. GDLs). (Josh Sole)

[1] Affiliated projects are team-based projects that involve GATE funded students and faculty but for which funding for the specific task is from a source other than the GATE Center.

- Development of characterization techniques for relative permeability in gas diffusion media. (Josh Sole)

B. Performance and durability modeling of PEM fuel cells

Engaged in research in the following areas related to modeling of PEM fuel cells:

- Development of models for the multi-scale, multi-physics characterization of reacting mixture flows in the micro-structures of PEMFC electrode catalyst layers using quantum thermodynamics (Charles Smith)
- Development of analytical models of the GDL that incorporate experimentally determined liquid transport characteristics. (Josh Sole)
- Development of strength based PEM durability model. *(Affiliated project)*

C. Fuel cell systems synthesis/design and control/operation optimization

Engaged in research in the following areas related to system design and optimization:

- Development of transient performance models for a hydrogen fuel cell APU (Bryan Shevock)

D. Fuel Cell and Hybrid Electric Vehicle energy use and environmental impact

- Analysis of the environmental characteristics of an advanced technology/alternative fueled vehicle fleet including hydrogen and fuel cell vehicles (Jeongwoo Lee) *(Affiliated project)*
- Vehicle Inertia Impact on Fuel Consumption using Pulse and Glide (Acceleration and Coast) Driving Strategy (Jeongwoo Lee)
- Plug-in hybrid vehicles using grid electricity, hydrogen and E85 fuels

E. Student progress on research projects

- Josh Sole: completed PhD dissertation "Investigation of Water Transport Parameters and Processes in the Gas Diffusion Layer of PEM Fuel Cells," May 2008.
- Charles Smith: continuing PhD on "Micro-structures of PEMFC Electrode Catalyst Layers Using Quantum Thermodynamics".
- Jeongwoo Lee: continuing PhD on "Vehicle Inertia Impact on Fuel Consumption".
- Bryan Shevock: completed MS on "Systems Level Transient Modeling of a Fuel Cell Auxiliary Power Unit", January 2008.
- Kurt Johnson: completed MS thesis on "A Plug-in Hybrid Electric Vehicle Loss Model to Compare Well-to-Wheels Energy Use from Multiple Sources", July 2008.

III. TASK 3 - STUDENT RECRUITMENT AND GATE FELLOWS SUPPORT

- Provided support for Bryan Shevock who completed his MS at the end of fall 2007.
- Provided support for Chris Fox who is working toward his MS and is investigating PEMFC membranes to determine material properties that lead to early failure by shorting.

– Provided support for GATE fellows, Charles Smith, started Spring 2007, and Kurt Johnson, started Summer 2007, with research topics as outlined in the previous section. Kurt Johnson completed his MS Thesis Summer 2008.

IV. TASK 4 - DISSEMINATION

A. Publications:

1. Arsalis, A., Calise, F., von Spakovsky, M.R., 2007, "Thermoeconomic Modeling and Parametric Study of Hybrid Solid Oxide Fuel Cell – Gas Turbine – Steam Turbine Power Plants Ranging from 1.5 MWe to 10 MWe," *Journal of Fuel Cell Science and Technology*, ASME, N.Y., N.Y., accepted for publication.
2. Arsalis, A., F. Calise, M.R. von Spakovsky, 2007, "Thermoeconomic Modeling and Parametric Study of Hybrid Solid Oxide Fuel Cell – Gas Turbine – Steam Turbine Power Plants Ranging from 1.5 MWe to 10 MWe," *Fourth International Conference on Fuel Cell Science, Engineering and Technology*, ASME, paper number: FUELCELL2007-25207, N.Y., N.Y., June.
3. Asinari, P., M. Calì Quaglia, M.R. von Spakovsky, and B.V. Kasula, 2007, "Direct Numerical Calculation of the Kinematic Tortuosity of Reactive Mixture Flow in the Anode Layer of Solid Oxide Fuel Cells by the Lattice Boltzmann Method," *Journal of Power Sources*, vol. 170, pp. 359-375.
4. Boyd, Steven , and Douglas J. Nelson, 2008, "Hybrid Electric Vehicle Control Strategy Based on Power Loss Calculations", SAE paper 2008-01-0084, *2008 SAE International World Congress*, April 14-17, 2008, Detroit, Mi, 15 pgs.
5. Calise, F., M.D. d' Accadia, L. Vanoli, M.R. von Spakovsky, 2007, "Full Load Synthesis/Design Optimization of a Hybrid SOFC-GT Power Plant," *Energy: The International Journal*, vol. 32, no. 4, p 446-458.
6. Cano-Andrade, S., A. Hernandez-Guerrero, M.R. von Spakovsky, C. Rubio-Arana, 2007, "Effect of Radial Plate Flow Field Distribution on Current Density in a Proton Exchange Membrane (PEM) Fuel Cell," *International Mechanical Engineering Congress and Exposition – IMECE'2007*, ASME Paper No. IMECE2007-42429, N.Y., N.Y., November.
7. Cano-Andrade, S., A. Hernandez-Guerrero, M.R. von Spakovsky, 2008, "Current Density Curves for Radial Configuration PEMFCs," *Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'08)*, Cracow, Poland, ASME, June 24-27.
8. Coppo, M., N.P. Siegel, M.R. von Spakovsky, 2007, "On the Influence of Temperature on PEM Fuel Cell Operation," *Journal of Power Sources*, Elsevier Press, Vol. 159/1, pp 560-569.
9. Dillard, D.A., Y.Q. Li, J.R. Grohs, S.W. Case, M.W. Ellis, Y.H. Lai, M. Budinski, C. Gittleman, "On the Use of Pressure-Loaded Blister Tests to Characterize the Strength and Durability of Proton Exchange Membranes," *ASME Journal of Fuel Cell Science and Technology* (*ASME-JFCST)*, accepted October 2007.
10. Grohs, Jacob R., Yongqiang Li, David A. Dillard, Scott W. Case, Michael W. Ellis, Yeh-Hung Lai, Michael Budinski, Craig Gittleman, "Evaluating the time and temperature dependent biaxial strength of Gore-Select® series 57 proton exchange membrane using a

pressure loaded blister test," *ASME Journal of Fuel Cell Science and Technology*, submitted October, 2007.

11. Johnson, Kurt, D.J. Nelson, 2009, "Design process and component sizing for range and performance goals in a series plug-in hybrid electric vehicle," to be submitted for EVS 24 May, 2009.
12. Kasula, B. V., L. Mercado, P. Asinari, M.R. von Spakovsky, 2007, "3D Microstructure Reconstructions of Solid Oxide and Proton Exchange Membrane Fuel Cell Electrodes with Applications to Numerical Simulations of Reacting Mixture Flows Using LBM," *International Mechanical Engineering Congress and Exposition – IMECE'2007*, ASME Paper No. IMECE2007-42937, N.Y., N.Y., November.
13. Kim, K., M. Wang, M.R. von Spakovsky, D.J. Nelson, 2008, "Dynamic Synthesis/Design and Operation/Control Optimization under Uncertainty of a PEMFC System," *International Mechanical Engineering Congress and Exposition – IMECE'2008*, ASME Paper No. IMECE2008-68070, N.Y., N.Y., Oct.-Nov.
14. Kim, K., M. Wang, M.R. von Spakovsky, D.J. Nelson, 2008, "Stochastic Modeling and Uncertainty Analysis with Multi-objective Optimization Strategies for the Synthesis/Design and Operation/Control of a PEMFC Fuel Processing Subsystem," *International Mechanical Engineering Congress and Exposition – IMECE'2008*, ASME Paper No. IMECE2008-68065, N.Y., N.Y., Oct.-Nov.
15. Lee, Jeongwoo Lee, D.J. Nelson, Henning Lohse-Busch, 2009, "Vehicle Inertia Impact on Fuel Consumption of Conventional and Hybrid Electric Vehicles Using Acceleration and Coast Driving Strategy," submitted for publication at *SAE International Congress* April 20-23, 2009.
16. Li, Yongqiang, J.K. Quincy, S.W. Case, M.W. Ellis, D.A. Dillard, Yeh-Hung Lai, M.K. Budinski, C.S. Gittleman, "Characterizing the Fracture Resistance of Proton Exchange Membranes," *Journal of Power Sources*, accepted May 2008.
17. Mazumder, S.K., S. Pradhan, J. Hartvigsen, M.R. von Spakovsky, D. Rancruel, 2007, "Effects of Battery Buffering and Inverter Modulation on the Post Load-Transient Performance of a Planar Solid-Oxide Fuel Cell," *IEEE Transactions on Energy Conversion*, IEEE, vol. 22, issue 2.
18. Mazumder, S.K., S. Pradhan, J. Hartvigsen, D. Rancruel, M.R. von Spakovsky, M. Kahleel, 2008, "A Multidiscipline and Multi-rate Modeling Framework for Planar Solid-oxide-fuel-cell based Power-Conditioning System for Vehicular APU," *Transactions of the Society for Modeling and Simulation*, SMS, September, in press.
19. Patankar, K.A., D.A. Dillard, S.W. Case, M.W. Ellis, Y.H. Lai, M.K. Budinski, C.S. Gittleman, "Hygrothermal Characterization of the Viscoelastic Properties of Gore® Select 57 Proton Exchange Membrane," *Mechanics of Time Dependent Materials*, accepted June 2008.
20. Pestrak, M., Y.Q. Li, S.W. Case, D.A. Dillard, M.W. Ellis, Yeh-Hung Lai, C.S. Gittleman, "The Effect of Catalyst Layer Cracks on the Fatigue Lifetimes of MEA," *6th International Conference on Fuel Cell Science, Engineering, and Technology*, 2008.
21. Shevock, Bryan and Douglas J. Nelson , 2008, "System Level Transient Model of a Fuel Cell System", SAE paper 2008-01-0636, *2008 SAE International World Congress*, April 14-17, 2008, Detroit, Mi, 17 pgs.

22. Smith, C. E., M.R. von Spakovsky, 2007, "Time Evolution of Entropy in a System Comprised of a Boltzmann Type Gas: An Application of the Beretta Equation of Motion," *International Mechanical Engineering Congress and Exposition – IMECE'2007,* ASME Paper No. IMECE2007-42933, N.Y., N.Y., November.
23. Smith, C. E., V. Verda, M.R. von Spakovsky, 2008, "Quantum Thermodynamics for the Modeling of Non-equilibrium Phenomena," *Efficiency, Costs, Optimization, Simulation and Environmental Aspects of Energy Systems (ECOS'08),* keynote address, Cracow, Poland, ASME, June 24-27.
24. Sole, Joshua D., M.W. Ellis, D.A. Dillard, "Experimental and analytical study of gas diffusion layer materials for ribbon fuel cells," *ASME Journal of Fuel Cell Science and Technology*, accepted November 2007.
25. Sole, Joshua D., M.W. Ellis, "Determination of the Relationship between Capillary Pressure and Saturation in PMEFC Gas Diffusion Media," *6th International Conference on Fuel Cell Science, Engineering, and Technology*, 2008.
26. von Spakovsky, M.R., C.E. Smith, V. Verda, 2008, "Quantum Thermodynamics for the Modeling of Hydrogen Storage on a Carbon Nanotube," *International Mechanical Engineering Congress and Exposition – IMECE'2008,* ASME Paper No. IMECE2008-67424, N.Y., N.Y., Oct.-Nov.
27. Wang, M., K. Kim, M.R. von Spakovsky, D.J. Nelson, 2008, "Multi- versus Single-Level Dynamic Synthesis/Design and Operation/Control Optimizations of a PEMFC System," *International Mechanical Engineering Congress and Exposition – IMECE'2008,* ASME Paper No. IMECE2008-68073, N.Y., N.Y., Oct.-Nov.
28. Wang, M., K. Kim, M. R. von Spakovsky, D.J. Nelson, 2008, "Use of State Space in the Dynamic Synthesis/Design and Operation/Control Optimization of a PEMFC System," *International Mechanical Engineering Congress and Exposition – IMECE'2008,* ASME Paper No. IMECE2008-68076, N.Y., N.Y., Oct.-Nov.
29. Verda, V., M.R. von Spakovsky, 2007, "2D Detailed Planar SOFC CFD Model for Predicting the Effects of Cell Performance Degradation," *Journal of Fuel Cell Science and Technology*, ASME, N.Y., N.Y., accepted for publication.

Other papers are in process for each of our research projects.

B. Professional Meetings:

1. Michael Ellis was the chair of the Systems Analysis and Fuel Cell Committee of the American Society of Mechanical Engineers.
2. Michael Ellis was Session Chair for *ASME International Mechanical Engineering Conference and Exhibition*, Seattle, WA, November 2007.
3. Michael Ellis was the Conference Organizing Committee for *6th International ASME Conference on Fuel Cell Science, Engineering and Technology*, Denver, CO, June 2008.
4. Michael Ellis was the Track Chair of the *ASME IMECE 2008,* Boston, MA, November 2008.
5. Michael Ellis is chair of the *7th International Conference on Fuel Cell Science, Engineering and Technology* to be held in Newport Beach, CA June 2009.

V. TASK 5 - INDUSTRY INTERACTION

A. Faculty and student attendance at industry forums:

Faculty and students from the Virginia Tech GATE Center attended many events during the period including 2008 Challenge X; 2008 SAE Congress, Detroit, MI; 2008 6th International Fuel Cell Science; Engineering and Technology Conference, Denver, CO. The Virginia Tech GATE Center also hosted visits from many automotive industry representatives during the past year.

B. Research project collaboration with automotive companies

- Michael Ellis, Chris Fox and Jessica Wright (undergraduate researcher) participated in bi-weekly web-meetings with other VT researchers and GM researchers working on PEM membrane research.
- Michael Ellis and Jessica Wright and Faculty (Dr. D.A. Dillard and Dr. S.W. Case) visited GM's Fuel Cell research facilities for a project review.

C. Research project presentations to government organizations

Doug Nelson attended and presented at the DoE Merit Review meeting on 28 February 2008.

D. Campus Visits by Industry

- Dr. Yeh-Hung Lai, General Motors Fuel Cell Research
  - Research collaboration
  - Seminars for REU students: Overviews of PEM Durability
  - Research Presentation: Viscoelestic Framework for Durability of PEM Materials
- Mr. Charles Strickler, Ecolectrix, LLC
  - Research collaboration
- Mr. Conal Deedy, Volvo Technology of America and Powercell Sv AB
  - Research proposal collaboration
- Luna Innovations, Inc.
  - Research on materials development for micro-tubular fuel cells for micro-air vehicles
- Dr. Ann Norris, Dow Corning Corporation
  - Discussion of possible collaborative research projects related to PEMFC's
- Ed Koerner, GM Vice President GM North America Engineering
  - Met with ME dept head and faculty to discuss automotive related curriculum and student projects and to identify opportunities for collaboration with GMGM

E. Graduate Students hired in fuel cell and/or automotive field[2]

- Kurt Johnson (MS): GM, June 2008
- Yongquiang Li (Ph.D.): GM FCA, 2008
- Bryan Shevock (MS): GM, HEV integration, February 2008
- Will Smith: ETEK, June 2007
- Meng Wang (Ph.D.): GM, FCA, December 2007

[2] Includes students supported directly by GATE and students working on GATE affiliated projects

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GATE Center for Automotive Fuel Cell Systems at Virginia Tech

DE-FG26-05NT42615

Progress Summary
Year Two 10/1/2006 – 9/30/2007
October 31, 2007

I. TASK 1 – CURRICULUM DEVELOPMENT

A. Taught ME 4015/4016: Engineering Design and Project, Fall 2006 and Spring 2007 to 27 Mechanical Engineering seniors, which included development of a demonstration hydrogen fuel cell APU module. This effort is continuing for ME 4015/4016 for Fall 2007 and Spring 2008 with 25 students.

B. Taught ME 4554 Advanced Technology Vehicles to 50 advanced undergraduate and graduate students in Fall 2006, where we covered performance and fuel economy modeling of fuel cell hybrid vehicles. This effort is continuing for ME 4554 for Fall 2007 with 46 students.

C. Prepared for ME 5254: Fuel Cell Systems and taught to 14 advanced undergraduate and graduate students in Spring 2007. This course was taught each spring from 2004 to 2006 by Michael Ellis. Doug Nelson will teach in spring 2008 and will expand the course content which addresses fuel cell systems for vehicles.

D. Taught ME4015/4016: Engineering Design and Project, Fall 2006 and Spring 2007, to 9 Mechanical Engineering seniors, which included the design, construction, and testing of a passive (with and without wicking) direct methanol fuel cell (DMFC) test fixture for testing 5 cm^2 membrane electrode assemblies (MEAs) based on Nafion™ or BPSH™.

II. TASK 2 – RESEARCH

A. Engaged in research in the following areas:
- Development of durability screening tests for PEM fuel cell membrane materials (Chris Fox)
- Analysis of the environmental characteristics of an advanced technology/alternative fueled vehicle fleet including hydrogen and fuel cell vehicles (Jeongwoo Lee)
- Development of transient performance models with validation for a hydrogen fuel cell APU (Bryan Shevock)
- Development of models for the multi-scale, multi-physics characterization of reacting mixture flows in the micro-structures of PEMFC electrode catalyst layers using quantum thermodynamics (Charles Smith)
- Set up testing for prototype novel hydride hydrogen generator (Kurt Johnson)

B. Progress on research theses and dissertations:
- Michael Christopher: completed MS thesis “Application of the Transient Hot-Wire Technique for Measurement of Effective Thermal Conductivity of Catalyzed Sodium Alanate for Hydrogen Storage”.

- Jungshik Baik: completed MS thesis “Experimental Investigation of the Effect of Composition on the Performance and Characteristics of PEM Fuel Cell Catalyst Layers”.
- Josh Sole: completed PhD preliminary presentation “Investigation of Water Transport Parameters and Processes in the Gas Diffusion Layer of PEM FuelCells”.
- Charles Smith: beginning PhD on “Micro-structures of PEMFC electrode catalyst layers using quantum thermodynamics”.
- Bryan Shevock: completing MS on “Validated PEMFC System Model”.

C. Research by GATE Center faculty members and GATE affiliated students have addressed the following topics:

- Characterization of the viscoelastic properties of PFSA membranes – Development of a constitutive model for PFSA viscoelastic properties. *(Affiliated project)*
- Characterization of the fracture energy of PFSA membranes using a knife slit test. *(Affiliated project)*
- Evaluation of the biaxial strength of PFSA membranes using pressure loaded blister tests. *(Affiliated project)*
- Simultaneous measurement of water uptake and strain in PFSA membranes. (Will Smith)

D. Research conducted in conjunction with industrial sponsorship by GATE Center faculty members and GATE affiliated students has addressed the following topics:

- Improvement of fuel cell performance, particularly at high current density, requires an understanding of liquid water transport in gas diffusion media.
- Development of characterization techniques for capillary pressure-saturation curves for materials of mixed wetability (i.e. GDLs). *(Josh Sole)*
- Development of characterization techniques for relative permeability in gas diffusion media. *(Josh Sole)*
- Development of analytical models of the GDL that incorporate experimentally determined liquid transport characteristics. *(Josh Sole)*

III. TASK 3 - STUDENT RECRUITMENT AND GATE FELLOWS SUPPORT

- Provided support for Will Smith who is working to complete his MS thesis.
- Provided support for Bryan Shevock who should complete his MS at the end of Fall 2007.
- Provided support for Chris Fox who is working toward his MS and is investigating PEMFC membranes to determine material properties that lead to early failure by shorting.
- Recruited two new GATE fellows, Charles Smith, starting Spring 2007, and Kurt Johnson, starting Summer 2007, with research topics as outlined in the previous section.

IV. TASK 4 - DISSEMINATION

A. Publications:

1. Y. Li, J. Quincy, D.A. Dillard, S.W. Case, M.W. Ellis, Y.H. Lai, M. Budinski, C. Gittleman, "Using a knife slitting test to characterize the fracture resistance of proton exchange membranes," *Proceedings of 4th International Conference on Fuel Cell Science, Engineering, and Technology*, June 19-21, 2006, Irvine, CA, Paper No. 97096.
2. Terpenny, J., Dancey, C., Goff, R., Nelson, D., Ellis, M., and Hong, D., AC 2007-2375: "Success Strategies for Capstone Design Courses with Large Classes, Diverse Project Types, Small to Large Student Teams, and Varied Faculty Interests and Approaches", Division: Design in Engineering Education Division, *2007 ASEE Annual Conference & Exposition*, Hawaii, June 24-27, 2007.
3. W. Smith, M.W. Ellis, S.W. Case, D.A. Dillard, Y.H. Lai, M. Budinski, C. Gittleman, "Simultaneous Measurement of Water Uptake and Strain in PFSA Membranes for Fuel Cells", *5th International Fuel Cell Science, Engineering, and Technology Conference*, June 18-20, 2007, New York City, Paper No. FuelCell2007-25316.
4. J.D. Sole, M.W. Ellis, D.A. Dillard, "Experimental and Analytical Study of Gas Diffusion Layer Materials for Ribbon Fuel Cells", *5th International Fuel Cell Science, Engineering, and Technology Conference*, June 18-20, 2007, New York City, Paper No. FuelCell2007-25206.
5. Y. Li, J. Grohs, S.W. Case, M.W. Ellis, D.A. Dillard, Y.H. Lai, M. Budinski, C. Gittleman, "Evaluating the Biaxial Strength of Proton Exchange Membranes using Pressure-Loaded Blister Tests", *5th International Fuel Cell Science, Engineering, and Technology Conference*, June 18-20, 2007, New York City, Paper No. FuelCell2007-25238.
6. K. Patankar, Y. Li, M.W. Ellis, S.W. Case, D.A. Dillard, Y.H. Lai, M. Budinski, C. Gittleman, "Characterizing the Viscoelastic Properties of Proton Exchange Membranes and Developing a Constitutive Model", *5th International Fuel Cell Science, Engineering, and Technology Conference*, June 18-20, 2007, New York City, Paper No. FuelCell2007-25211.
7. Shannon Geiger (Advisor- Michael Ellis), poster presentation, "Effects of Microporous Sublayer Loadings on PEM Fuel Cell Performance", *23rd Annual Virginia Tech Graduate Research Symposium*, Awarded 1st Place for Advanced Undergraduate Research.
8. Asinari, P., Calì Quaglia, M., von Spakovsky, M.R., and Kasula, B.V., 2007, Direct Numerical Calculation of the Kinematic Tortuosity of Reactive Mixture Flow in the Anode Layer of Solid Oxide Fuel Cells by the Lattice Boltzmann Method, *Journal of Power Sources*, vol. 170, pp. 359-375.
9. Mazumder, S.K., Pradhan, S, Hartvigsen, J., von Spakovsky, M. R., Rancruel, D., 2007, Effects of Battery Buffering and Inverter Modulation on the Post Load-Transient Performance of a Planar Solid-Oxide Fuel Cell, *IEEE Transactions on Energy Conversion*, IEEE, vol. 22, issue 2. June 2007, pp. 457 – 466.
10. Pradhan, S, Mazumder, S.K., Rancruel, D., von Spakovsky, M.R., Hollist, M., Hartvigsen, J., Kahleel, M., 2007, A Modeling Framework for Planar Solid Oxide Fuel Cell based Power Conditioning System for Vehicular APUs, *IEEE Transactions on Power Electronics*, IEEE Power Electronics Society, special issue on Automotive Power Electronics & Motor Drives, in press.

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17. Jih-Sheng (Jason) Lai, and Douglas J. Nelson, "Energy Management Power Converters in Hybrid Electric and Fuel Cell Vehicles", (invited) accepted for the IEEE Proceedings special issue on *Electric, Hybrid & Fuel Cell Vehicles.*

Other papers are in process for each of our research projects.

Abstract titled, "Experimental and Analytical Study of Gas Diffusion Layer Materials for Ribbon Fuel Cells" prepared by Josh Sole was accepted for presentation at the Fifth International Conference on Fuel Cell Science, Engineering, and Technology. Full paper has been submitted to a special conference edition of the *ASME Journal of Fuel Cell Science and Technology*.

B. Professional Meetings:

1. Michael Ellis and Will Smith participated in bi-weekly web-meetings with other VT researchers and GM researchers working on PEM membrane research.

2. Doug Nelson taught the SAE Professional Development seminar, "Automotive Fuel Cell Systems" in March and August 2007 to 25 automotive industry professionals.

3. Michael von Spakovsky taught Techniques for the Modeling, Analysis, and Optimization of High and Low Temperature Fuel Cells: From the Microscopic Level to the System Level short course twice in 2006.

4. Michael Ellis was the chair of the Systems Analysis and Fuel Cell Committee of the American Society of Mechanical Engineers. He organized a conference

session on Fuel Cell Systems for the 2006 ASME International Mechanical Engineering Congress and Exhibition.

C. Public Forums:

1. Several posters were presented at the 2006 Dean's Forum on Energy Security and Sustainability:
    - http://www.research.vt.edu/energy/Hydrogen_Fuel_Cells_Poster_Abstracts.html including: "Hydorgen Fuel Cell Auxiliary Power Unit for Transportation Applications"
    - "Advanced Technology Vehicle Fleet Impact Assessment Study" (including H2 and FCVs), "Multi-physics, Multi-scale Models: Low and high Temperature Fuel Cells"
    - "System/Component Modeling/Optimization for Fuel Cell System Synthesis/Design and Operational/Control"

2. Congressman Rick Boucher attended Dean's Forum on Energy Security and Sustainability, observed our fuel APU project, and drove our Challenge X hybrid electric vehicle.

3. Association of Energy Conservation Professionals, displayed running fuel cell auxiliary power unit and poster for the public at the conference, Dec. 1-2, 2006, Roanoke, Va.

V. TASK 5 - INDUSTRY INTERACTION

A. Faculty and students from the Virginia Tech GATE Center attended many events during the period, including 2006 ASME IMECE, 2006 SAE Congress, 2006 Challenge X, 2006 Challenge Bibendum, the Virginia Hydrogen Economy Roundtable, 2007 SAE Congress, 5th International Fuel Cell Science, Engineering, and Technology Conference, June 18-20, 2007, 2007 Challenge X.. The Virginia Tech GATE Center also hosted visits from many automotive industry representatives during the past year.

B. Michael Ellis, Will Smith, and Chris Fox participated in bi-weekly web-meetings with other VT researchers and GM researchers working on PEM membrane research.

C. Doug Nelson attended and presented at the DoE Merit Review meeting on 19 June 2007.

D. Campus Visits by Industry
- Dr. Craig Gittleman, General Motors Fuel Cell Research
    - Presented seminar "Proton-Exchange Membranes for Automotive Fuel Cell Applications"
- Dr. Yeh-Hung Lai, General Motors Fuel Cell Research
    - Research collaboration
- Mr. Charles Strickler, Ecolectrix, LLC
    - Research collaboration
- Mr. Conal Deedy, Volvo Technology of America and Powercell Sv AB
    - Research proposal collaboration

E. Students hired in fuel cell or automotive field[1]
   - Tommy Coupar (BS): Ford Motor Company
   - Jungshik Baik (MS): LG Electronics
   - Li Yongqiang (PhD in progress): General Motors
   - Chris Fox
   - Will Smith (MS in progress): ETEK
   - Josh Sole
   - Kurt Johnson (MS in progress): General Motors
   - Bryan Shevock (MS in progress): General Motors
   - Charles Smith

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Faculty Advisor, Hybrid Electric Vehicle Team of VA Tech
http://www.me.vt.edu/hevt

[1] Includes students supported directly by GATE and students working on GATE affiliated projects

GATE Center for Automotive Fuel Cell Systems at Virginia Tech

DE-FG26-05NT42615

Progress Summary
Year One 10/1/2005 – 9/30/2006
July 31, 2006

TASK 1 - Curriculum development

Taught ME 4015/4016: Engineering Design and Project to 30 Mechanical Engineering seniors, which included development of a demonstration hydrogen fuel cell APU module.
Taught ME 4554 Advanced Technology Vehicles to 50 advanced undergraduate and graduate students in Fall 2005, where we covered performance and fuel economy modeling of fuel cell hybrid vehicles.
Continued revision of ME 5254: Fuel Cell Systems to use a new textbook and taught 16 advanced undergraduate and graduate students in Spring 2006.
Revised and taught ME 4984/ME 5984: Hydrogen Energy Systems to 22 advanced undergraduate and graduate students in Spring 2006.

TASK 2 – Research

Engaged in research for hydrogen storage using sodium alanate hydride system, PEM material characterization of the response of fuel cell membrane materials to temperature and moisture, and advanced technology/alternative fueled vehicle fleet environmental studies including hydrogen and fuel cell vehicles.

TASK 3 - Student Recruitment and GATE Fellows Support

Provided partial support for Mike Christopher who completed his MS at the end of Spring 2006.
Provided support for Will Smith who will complete his MS thesis at the end of Fall 2006.
Due to the start date, we did not fund as many GATE Fellows as planned for Year One, but intend to use the unobligated balance from Year One to fund an additional GATE Fellow in Year Two.
Recruited the best students to GATE from our NSF Research Experiences for Undergraduates and our Graduate Student Weekend events. We expect to have 4 GATE fellows for 2006-2007.

TASK 4 - Dissemination

Doug Nelson taught the SAE Professional Development seminar, "Automotive Fuel Cell Systems" in March and August 2006 to 27 automotive industry professionals.
Mike Ellis and Will Smith participate in bi-weekly web-meetings with other VT researchers and GM researchers working on PEM membrane research.
Mike Ellis is currently the chair of the Systems Analysis and Fuel Cell Committee of the American Society of Mechanical Engineers. He is organizing a session on Fuel Cell Systems for the upcoming 2006 ASME International Mechanical Engineering Congress and Exhibition.

Y. Li, J. Quincy, D.A. Dillard, S.W. Case, M.W. Ellis, Y.H. Lai, M. Budinski, C. Gittleman, "Using a knife slitting test to characterize the fracture resistance of proton exchange membranes," *Proceedings of 4th International Conference on Fuel Cell Science, Engineering, and Technology*, June 19-21, 2006, Irvine, CA, Paper No. 97096.
Other papers are in process for each of our research projects.

TASK 5 - Industry Interaction

Faculty and students from the Virginia Tech GATE Center attended many events during the period, including 2005 ASME IMECE, 2006 SAE Congress, 2006 Challenge X, 2006 Challenge Bibendum, and the Virginia Hydrogen Economy Roundtable. The Virginia Tech GATE Center also hosted visits from many automotive industry representatives during the past year.