



# U.S.-CHINA CLEAN ENERGY RESEARCH CENTER 中美清洁能源研究中心

## ANNUAL REPORT 2012-2013

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Accomplishments from the Second Year of  
the U.S.-China Clean Energy Research Center

*The United States and China share strategic and economic interests in advancing clean energy technologies. Our futures depend on the efficient use and innovative production of clean fuels and power.*

*Innovative technologies vital to the energy strategies of both our countries are now under development at the U.S.-China Clean Energy Research Center (CERC). These technologies will help to assure clean and efficient energy futures; reduce vulnerabilities to oil disruptions and the cost of imports; improve air quality, especially in and around growing population centers; and strengthen economic growth. These technologies will also help to mitigate the impacts of energy production and use on the global environment.*

*Having now completed the second year of its initial five-year plan, CERC serves as a proven model for enhanced cooperation on technology research and development (R&D). With encouragement and support from both governments, CERC provides a platform for nurturing productive new alliances among some of the world's most knowledgeable and creative innovators in academia and industry. Teams of CERC scientists and engineers jointly plan and carry out collaborative R&D that leverages the complementary strengths of each country.*

*U.S. President Barack Obama and China President Hu Jintao first announced this bilateral, flagship initiative in November 2009, and the U.S.-China CERC was officially launched with the signing of joint work plans and technology management plans in 2011. Since then, President Obama and China's current President Xi Jinping have affirmed their intentions to continue useful bilateral cooperation on clean energy innovation—including CERC.*



U.S. president Barack Obama and China president Xi Jinping endorse a new model for U.S.-China cooperation.

# Contents

Message from CERC Directors .....	v
Executive Leadership .....	vi
Introduction .....	1
CERC Accomplishments in Year 2 .....	3
Advanced Coal Technology Consortium.....	4
Building Energy Efficiency Consortium.....	8
Clean Vehicles Consortium.....	12
Intellectual Property Framework .....	16
Conclusions and Future Plans .....	20
Appendix A: Maps of Consortia Partner Locations .....	A1
Appendix B: CERC Organizational Structure .....	B1
Appendix C: CERC Funding.....	C1
Appendix D: Procedures for Adding New Members.....	D1
Appendix E: Advanced Coal Technology Consortium Project Fact Sheets.....	E1
Appendix F: Building Energy Efficiency Consortium Project Fact Sheets .....	F1
Appendix G: Clean Vehicles Consortium Project Fact Sheets .....	G1
Appendix H: Acronym List .....	H1





## Message from CERC Directors

This is the 2<sup>nd</sup> Annual Report on the progress of the U.S.-China Clean Energy Research Center. As the Center approaches the mid-point in its initial 5-year commitment period, this Report takes stock of accomplishments; assesses progress to date, both in terms of bilateral cooperation and technical achievement; and plots a course for the future.

The goal of the joint Center is to accelerate the development and deployment of clean energy technologies for the benefit of both countries. The key idea is to do this better, faster, and cheaper by working together. The Center enables and encourages top scientists and engineers in both countries to join forces, learn from each other, and build on complementary strengths. Teams jointly plan projects, attract industry partners, parse tasks, divide labor, leverage resources, take on more work, and speed progress.

The Center is pursuing three technical tracks that together account for 88 projects, of which more than two-thirds are joint. It supports 1,100 researchers and has 110 partners. An independent review found the Center to be a “milestone initiative” that is “pragmatic” and “win-win.” The review indicated that the Center “enables a new kind of relationship, built on mutual trust, understanding, and friendship.”

Although it is too early to gauge fully the Center’s impact, benefits are beginning to be seen with significant outcomes in all three tracks. The advanced coal technology teams, for example, are producing innovations that will bring cleaner, more efficient, and affordable electric power to consumers. This year, they developed new techniques, tools, and processes that reduce energy consumption, decrease costs, and reduce emissions.

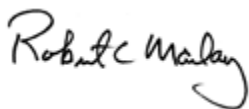
The building energy efficiency teams are developing innovative tools and technologies that will enable citizens to live and work in more comfortable, energy-efficient buildings. This year, they developed improved building envelope materials, standards, and tools, and improved the efficiency of climate control systems.

Clean vehicles teams are creating innovations that will enable citizens to drive in safe, lightweight vehicles that use less fuel or alternative fuels such as electricity and bio-fuels. This year, they developed novel cathode designs, new materials, and improved simulation tools that will enhance battery performance and inform battery and vehicle body design.

The Center continued to strengthen its groundbreaking framework for the protection of intellectual property. The government-backed technology management plans enable partners to bring forward their best ideas with confidence that IP rights will be protected.

Business interest in the Center is rising. Industrial partners contribute meaningful resources and guide R&D planning. Business ventures explore ways to collaborate, share data, demonstrate advanced technology, expand markets, and accelerate deployment. Additional partners seek to join. Guidelines for their entry have been approved by both countries. This broad-based and inclusive approach is helping the Center grow strategically.

Any successes the Center has achieved to date must be attributed to its technical leaders and their research teams. We salute their creativity, hard work, and willingness and commitment to work collaboratively across long distances, two cultures, and different languages to make this idea work and work well. We look forward to further progress that will, with continued success, position the United States and China as leaders in clean technology and innovation and move both countries toward a prosperous, clean, and energy-efficient future.



Dr. Robert C. Marlay, Ph.D  
Center Director for the United States  
U.S. Department of Energy



Counselor Liu Zhiming, Ph.D  
Center Director for the People’s Republic of China  
Ministry of Science and Technology

# Executive Leadership

## *Steering Committee Members*

Dr. Ernest Moniz  
Secretary  
U.S. Department of Energy

Dr. Wan Gang  
Minister  
China Ministry of Science and Technology

Dr. Wu Xinxiang  
Administrator  
China National Energy Administration

Dr. Qiu Baoxing  
(Ex-officio) Vice Minister  
China Ministry of Housing and Urban-Rural Development

## *Secretariat*

Jonathan Elkind  
Acting Assistant Secretary for Policy and International Affairs  
U.S. Department of Energy

Cao Jianlin  
Vice Minister  
China Ministry of Science and Technology

Ma Linying  
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China Ministry of Science and Technology

Li Ye  
Chief Economist  
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Dr. Robert C. Marlay  
CERC Director  
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Counselor Liu Zhiming  
CERC Director  
China Ministry of Science and Technology

Dr. Casey Delhotal  
Director of East Asian Affairs  
U.S. Department of Energy

Wang Qiang  
Director, Americas and Oceania  
China Ministry of Science and Technology

## *Advanced Coal Technology Consortium*

Dr. Jerald J. Fletcher  
Director  
West Virginia University

Dr. Zheng Chugang  
Director  
Huazhong University of Science and Technology

Dr. S. Julio Friedmann  
Technical Program Manager  
Lawrence Livermore National Laboratory

Dr. Xu Shisen  
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Dr. Qingyun Sun  
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West Virginia University

Dr. Yao Qiang  
Chief Scientist  
Tsinghua University

Sam Taylor  
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West Virginia University

## *Buildings Energy Efficiency Consortium*

Dr. Nan Zhou  
Director  
Lawrence Berkeley National Laboratory

Liang Junqiang  
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Science and Technology Center, Ministry of Housing and Urban-Rural Development

Dr. Yuan Yao  
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Dr. Jiang Yi  
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Science and Technology Center, Ministry of Housing and Urban-Rural Development

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Founding Director and Advisor  
Lawrence Berkeley National Laboratory

Brian Heimberg  
Operations Manager  
Lawrence Berkeley National Laboratory

## *Clean Vehicles Consortium*

Dr. Hwei Peng  
Director and China Liaison  
University of Michigan

Dr. Ouyang Minggao  
Director  
Tsinghua University

Dr. Jun Ni  
Deputy Director and China Liaison  
University of Michigan

Dr. Wang Hewu  
Deputy Director  
Tsinghua University

Dr. Qiu Xinping  
Deputy Director  
Tsinghua University

Carrie Morton  
Operations Manager  
University of Michigan



# Introduction



## Common Ground on Energy Use and Production

The United States and China are the world's two largest economies, as well as the world's largest producers and consumers of energy. Our countries share many common challenges, interests, and perspectives related to energy use and production:

- China and the United States together account for 40% of annual global emissions of greenhouse gases.
- Both countries are highly dependent on coal for electricity—about 50% of the electricity generated in the United States and 80% in China is from coal.
- Both countries rely heavily on foreign sources of oil, importing more than 50%.
- Both countries recognize the vital importance of improving energy efficiency.
- Both countries are expanding and modernizing infrastructure, much of which has yet to be built and can be significantly influenced by advances in technology.
- Both countries see scientific discovery and innovation as means to inspire and spur economic growth and improve the quality of life of all citizens.
- Both countries have vast intellectual capacities for solving big problems.

*The United States and China have a history of positive, cooperative collaboration on science and technology (S&T) development. Despite different political systems, historical and cultural backgrounds, and levels of economic development for the past 30 years, the United States and China have established a new era of S&T cooperation in diverse disciplines. In the field of clean energy, the United States and China are working together on dozens of programs in a groundbreaking research initiative to advance technologies that provide energy and environmental benefits for both countries.*

## Today's Challenges

As the world transitions to a clean energy economy, China and the United States—the world's top energy consumers and energy producers—clearly play important roles. Both countries are working to increase the generation and use of secure, affordable, and clean energy. In doing so, we face common challenges, such as climate change and environmental protection. Cooperation between our countries is critical in successfully addressing these issues.

The United States and China both have rapidly growing clean energy sectors that feature leading research institutes and innovative businesses. Both nations

recognize that advancing cooperative scientific discovery while effectively protecting intellectual property (IP) is a promising avenue to expand our foundation of knowledge, technology, and capacity—positioning both countries for a prosperous, clean, and energy-efficient future.

“CERC is a great model to promote cooperation between China and the United States. In the future, in addition to clean energy, it can be applied to agriculture, health, basic research and other areas of mutual interest.”

Liu Yandong  
China Vice Premier

## Vision of the U.S.-China Clean Energy Research Center

CERC accelerates the development and rapid deployment of critical technologies for cleaner use of coal, energy efficiency in buildings, and clean vehicles in the United States and China. These efforts are executed with the goal of generating a diversified energy supply and accelerating the transition to a low-carbon economy while avoiding the worst consequences of climate change.

CERC conducts cooperative activities on the basis of five principles:

- Equality, mutual benefit, and reciprocity
- Timely exchange of information relevant to cooperative activities
- Effective protection of intellectual property rights
- Peaceful, non-military uses of the results of collaborative activities
- Respect for the applicable legislation of each country

## Cooperation on Clean Energy Technologies Benefits Both Countries

As the world's two largest energy markets, the United States and China both benefit from clean energy innovations. Collaborative research strengthens domestic industries, ensuring that the two nations remain at the forefront of clean energy technologies. This market leadership creates jobs in both countries, generates exciting new products for consumers, and boosts exports.

More than 1,100 CERC researchers are collaborating on 88 projects, of which two thirds are joint, to help create an improved energy future by developing the following:

- Greater access to new markets for businesses, strengthening the economy and creating new jobs
- Innovative building technologies that save energy and improve comfort
- Cleaner and more efficient power that is generated with fewer emissions
- Advanced vehicles that are safe, save money, and reduce dependence on foreign oil

## Importance of Innovation

Given the importance of S&T to economic and social development, these disciplines have long served as a cornerstone of cooperation between the United States and China. Our countries share a responsibility to contribute to the world's future sustainability and prosperity by taking advantage of opportunities to cooperate in advancing clean energy technologies.

Collaborative research in the United States and China can spur rapid innovation. By learning from each other and working together to develop new technologies, our countries can maintain their lead roles in global innovation and create new export opportunities for partner companies. Discoveries in S&T lead to innovations, which often become powerful drivers for economic growth.

## A Landmark Initiative

Recognizing the importance of innovation and the energy challenges that the United States and China face together, the U.S.-China Clean Energy Research Center (CERC)

partnership advances common interests, addresses shared concerns, and highlights international responsibilities. CERC helps the United States and China meet energy and environmental goals by facilitating the research, development, and commercialization of clean energy technologies by teams of scientists and engineers in both countries. It also serves as a bilateral platform to increase access to specialized expertise and clean energy knowledge.

CERC's new model for enhanced S&T cooperation is grounded in the understanding that protecting IP is a vital part of driving innovation. By encouraging innovations to arise jointly, the model creates an attractive platform for collaborative research and business investment. It protects IP in a way that builds confidence among researchers and ensures that both the United States and China benefit from collective research. Through this pioneering model for U.S.-China clean energy cooperation, industry partners, research institutes, and government officials accelerate innovation in advanced coal, clean vehicles, and building energy efficiency.



Secretary Steven Chu and Minister Wan Gang at the January 2013 Steering Committee Meeting in Washington, DC.



# CERC Accomplishments in Year 2



## Industry Partners Are Central to CERC Success

Business and government research teams in both countries work together to accelerate innovation and commercial success. In contrast to traditional frameworks for collaboration, the CERC collaborative model offers industry partners several key benefits that empower them to assume a central role:

- Enhanced intellectual property protection
- Early and continuing involvement in the innovative process
- Insights into ongoing research processes
- Ownership or licensing of IP for commercial purposes
- Exposure to potentially large markets for new technologies

These benefits have successfully attracted active industry participation and support for CERC research efforts. Preeminent manufacturing and technology development firms are co-leading selected research projects, spearheading planning efforts and information exchanges, and providing essential funding that amplifies the research investments made by the U.S. and Chinese governments. CERC has successfully partnered with 110 businesses and NGOs with strong participation from both United States and China.

*The U.S.-China Clean Energy Research Center consortia grew to maturity in their second year of operation—spanning the latter part of 2012 and the first part of 2013. With endorsements from the highest levels of the U.S. and Chinese governments and support from forward-looking companies, CERC programs built strong teams of distinguished and creative scientists and technical leaders. Collaboration is the centerpiece of CERC, and its value cannot be overemphasized. These partnerships have yielded revolutionary, cross-governmental and cross-disciplinary research and development.*

In 2012-2013, CERC research teams actively leveraged their unique experimental platforms, data, and business relationships in each country. Buttressed by robust funding support and in-kind contributions, R&D planning is guided by industrial partners. The successes have piqued the interest of other private entities, and the number of private-sector partners has continued to grow. The coming years promise further developments from a growing roster of participants, and CERC welcomes companies and research partners ready to bring their strengths and contributions to bear on this exciting and dynamic endeavor.

## *Achievements of the Research Consortia*

All three research consortia—the Advanced Coal Technology Consortium, the Building Energy Efficiency Consortium, and the Clean Vehicles Consortium—can claim impressive technical breakthroughs. These technical advancements would not be possible without CERC's framework for protecting and sharing intellectual property that promotes open collaboration. Accomplishments of the three research consortia and advancements in IP are presented in the following sections.

# Advanced Coal Technology Consortium



## CERC Advanced Coal Technology Vision

Advance the coal technologies needed to safely, effectively, and efficiently utilize coal resources, including capture, storage, and utilization of emissions from coal use.

## Addressing Common Challenges Presents Opportunities to Deliver Mutual Benefits

The United States and China both possess abundant coal resources and are dependent on coal for electricity. The use of coal in electricity generation introduces challenges and opportunities in environmental performance and commercial development.

Advanced coal technology research supports the development of innovations that will bring cleaner, more efficient, and affordable electric power to consumers. It will help deliver essential technologies and practices:

- Cleaner processes for combusting coal to generate electricity
- More efficient power plants
- Technologies that can capture carbon dioxide (CO<sub>2</sub>) emissions and store them permanently
- Assessment of the geological formations to facilitate the permanent underground storage of CO<sub>2</sub> emissions
- Improved overall coal utilization efficiency with improved polygeneration systems

*The United States and China are collaborating through the Advanced Coal Technology Consortium (ACTC) to develop and deploy cleaner coal technologies and practices for capturing, storing, and utilizing carbon dioxide emissions. Jointly planned research through this collaboration is producing results that enable clean coal power plants to produce electricity at a lower cost and with lower carbon emissions, which will lead to economic development, reduced emissions, and improvement in the overall energy efficiency of coal utilization.*

ACTC projects have already resulted in 17 patents, 270 published papers, 80 conference presentations, and five memoranda of understanding between U.S. and Chinese companies. The ACTC platform for joint research focuses on the following eight research topics (see Appendix E for more detail on ACTC research activities):

1. Advanced Power Generation
2. Clean Coal Conversion Technology
3. Pre-Combustion CO<sub>2</sub> Capture
4. Post-Combustion CO<sub>2</sub> Capture
5. Oxy-Combustion Research, Development, and Demonstration
6. Sequestration Capacity and Near-Term Carbon Capture, Use, and Storage (CCUS) Opportunities
7. CO<sub>2</sub> Algae BioFixation and Use
8. Integrated Industrial Process Modeling and Additional Topics

Significant technical highlights from 2012-2013 efforts across the ACTC teams are provided on the following pages.

## Significant ACTC Joint Programmatic Activities in Year 2

ACTC leaders convened several productive program planning and strategy meetings in 2012-2013, including:

- All-hands meeting in Wuhan, China, to review progress made by Chinese researchers
- Joint meeting in Wuhan, China, to discuss progress on key collaborative efforts from both countries
- Intellectual Property workshop in Hainan, China, to discuss licensing and IP issues





# Key Achievements in Advanced Coal Technology

## Validated co-generation technology at pilot plant

Joint researchers working on clean coal conversion technologies have validated the modeling results on a 1 MW pilot plant for coal co-generation technology, which combines pyrolysis, gasification, and combustion. The co-generation technology is expected to reduce maintenance costs and greenhouse gas emissions by more than 25% compared to conventional technology.

Researchers are further developing the new co-generation system and advanced coal gasification processes and plan to demonstrate the technologies at industrial scale for development and sale in the United States and China. (Refer to page E5, Appendix E: ACTC research topic 2)

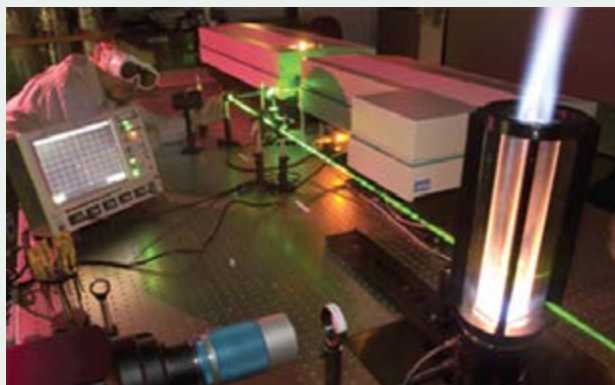


Demonstration of combined pyrolysis, gasification, and combustion at a 1 MW pilot plant illustrates the potential for cost savings and CO<sub>2</sub> emissions reductions.

## Improved modeling capabilities for oxy-combustion

Researchers characterized four U.S. and four Chinese coals and developed computational fluid dynamics (CFD) models for U.S. and China pilot-scale test facilities, leading to cost and performance improvements in oxy-firing combustion.

CERC partners in China and in the United States signed a research collaboration agreement in June 2012, and the joint research efforts are already producing advancements in computer simulation and modeling of oxy-firing combustion. The computer models, once validated at large scale commercial projects, will increase the rate of deployment for a wide variety of world coals using oxy-combustion technology that facilitates CO<sub>2</sub> capture. (Refer to page E10, Appendix E: ACTC research topic 5)



Flat-flame reactor with optics diagnosis provides data for models that can lead to significant improvements in oxy-combustion.

## Published significant findings on CO<sub>2</sub> storage

CERC researchers produced 11 peer-reviewed publications and conference papers on the storage and utilization of CO<sub>2</sub> in the Ordos Basin in China. Researchers initiated design, construction, and injection of CO<sub>2</sub> at a pilot CO<sub>2</sub>-enhanced oil recovery (EOR) project in the Ordos Basin. They also assembled a large data set regarding the geologic, petrophysical structural/stratigraphic frameworks of the Ordos Basin, as well as the Wyoming and Illinois Basins in the United States. The significant opportunity for storage and utilization of CO<sub>2</sub> in the Ordos Basin complements opportunities that are being explored in Wyoming and Illinois Basins. (Refer to page E12, Appendix E: ACTC research topic 6)



The Yanchang Oil Field in China's Ordos Basin, which is comparable to the Wyoming and Illinois Basins in the United States, holds substantial potential for CO<sub>2</sub> storage.



# Key Achievements in Advanced Coal Technology

## Post-combustion simulation yielded favorable cost estimates

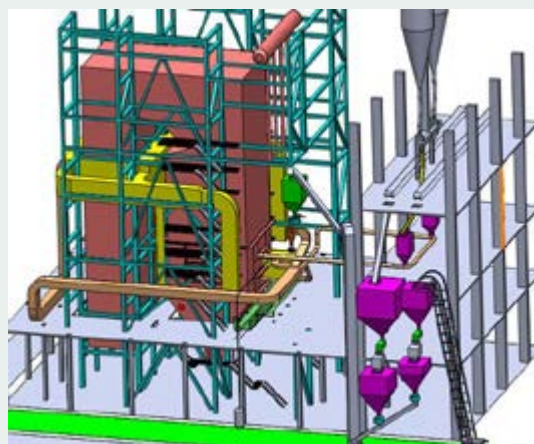
Researchers completed the simulation of a 1 million ton/year post-combustion CO<sub>2</sub> capture system, advancing new capture and solvent technologies for the development of efficient CO<sub>2</sub> capture in existing coal plant retrofits. This revealed advantages over other methods and suggested a cost of US\$61–\$68 per metric tonne at Duke's Gibson 3 plant in Indiana. CERC researchers simulated the post-combustion capture, mixed-amine absorption process at Shidongkou, allowing performance assessments under varying decision-making environments. A two-phase solvent and new catalyst family with record activity levels were also developed for the project. (Refer to page E8, Appendix E: ACTC research topic 4)



Many existing coal plants, such as the facility shown here, have the potential for CO<sub>2</sub> capture system retrofit.

## Novel coal-to-chemicals polygeneration simulated and ready for testing

CERC researchers completed experiments and simulations of a coal-to-chemicals polygeneration scheme of LP Amina's calcium-carbide reactor. The simulation findings will be used to design and build a very high temperature polygeneration reactor at lab scale. The results set the stage for improved operation and commercialization, with potential for scale-up in China's markets. New polygeneration technologies are expected to dramatically reduce waste heat, water use, and greenhouse gas emissions while improving thermal efficiency of power generation and chemical by-products production. (Refer to page E5, Appendix E: ACTC research topic 2)



Design options for next generation coal-to-chemicals technology demonstrates the integration of power generation and chemical production.

## Design configurations assessed for CO<sub>2</sub> utilization with microalgae

CERC researchers examining CO<sub>2</sub> utilization in algae growth systems optimized designs using a range of U.S. and Chinese strains under different reactor designs. The researchers are developing and demonstrating an economically feasible technology for CO<sub>2</sub> utilization with microalgae and transformation of algal biomass into a sustainable source of energy. Further assessments are ongoing at Duke Energy's East Bend power plant (see image at right). The accumulated data will be incorporated in a techno-economic model that will identify potential economies of scale. Collaborative research and data sharing is enabling the assessment of a range of process configurations, such as open pond cultivation and closed-loop photobioreactors. (Refer to page E14, Appendix E: ACTC research topic 7)



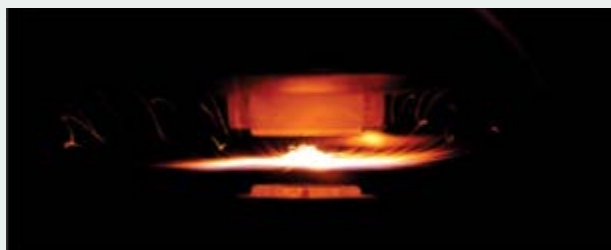
CERC researchers are exploring reactor designs for algae growth in a demonstration facility installed at Duke Energy's East Bend power plant at Rabbit Hash, Kentucky, United States.

# Key Achievements in Advanced Coal Technology

## First-of-a-kind experimental system developed

Researchers designed and constructed a unique experimental system to research pulverized coal combustion in counterflow flames and developed toolbox of energy conservation and emission reduction technologies for coal-fired power plants. Researchers investigated combustion characteristics of Xinjiang Houxun coal in advanced ultra supercritical (A-USC) boilers. Power plants equipped with A-USC boilers have the potential to dramatically improve efficiency and reduce emissions compared to existing coal-fired power plants. The development of improved A-USC boiler technologies was adopted as a national program in China.

A survey by CERC researchers found that, by the end of 2009, subcritical power plants accounted for 78% of China's coal-fired fleet, while supercritical and ultra supercritical units made up the remaining 22%. Researchers are targeting subcritical units in China and the United States with a capacity range of 300–600 MW to maximize system-wide impacts of plant efficiency improvements and emissions reductions potential. (Refer to page E3, Appendix E: ACTC research topic 1)



Particle behavior is examined during flame penetration of coal combustion.

## Energy penalty from post-combustion CO<sub>2</sub> capture reduced in simulation

Researchers simulated a steady-state scenario for CO<sub>2</sub> capture from a supercritical pulverized coal power plant using a monoethanol amine (MEA) solvent. Optimizing the design and operating parameters, researchers were able to reduce the simulated net energy penalty by 2.5%—from 12.7% to 10.2%.

Application of advanced modeling and simulation tools are helping enable improvements in technology and systems integration that are not otherwise possible due to the very complex nature of the interacting processes present in large-scale power generators with carbon capture. Such improvements are expected to decrease the cost and improve the performance of CO<sub>2</sub> capture technologies. (Refer to page E15, Appendix E: ACTC research topic 8)



Advanced modeling and simulations enable technology advancements to existing coal-fired systems.

## Advanced Coal Technology Consortium (ACTC) Partners

The U.S. ACTC is led by the **West Virginia University Research Corporation**. The U.S. Consortium includes the following partners:

- Babcock & Wilcox
- Duke Energy
- Indiana Geological Survey
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- LP Amina
- National Energy Technology Laboratory
- University of Kentucky
- University of Wyoming
- U.S.-China Clean Energy Forum, Washington State China Relations Council
- World Resources Institute

China's ACTC is led by **Huazhong University of Science and Technology**, based in Wuhan, and includes the following partners:

- China Huaneng Group Clean Energy Research Institute
- China Huaneng Group Power International, Inc.
- China Power Engineering Consulting Group Corporation (CPECC)
- China Power Investment Corporation
- China University of Mining and Technology
- ENN (XinAo Group)
- Harbin Institute of Technology
- Institute of Rock & Soil Mechanics, Chinese Academy of Science
- Northwest University of China
- Research Center for Energy and Power, Chinese Academy of Sciences
- Shaanxi Yanchang Petroleum (Group)
- Shanghai JiaoTong University
- Shenhua Group Corporation
- Tsinghua University
- Zhejiang University

# Building Energy Efficiency Consortium



## CERC Building Energy Efficiency Vision

To build jointly a foundation of knowledge, technologies, tools, human capabilities, and relationships to position the United States and China for a future with VLEBs, greatly reducing CO<sub>2</sub> emissions.

## Developing Innovative Building Energy Efficiency Technologies Benefit Both Countries

Considerable opportunities to improve building energy efficiency exist across the United States and China. In the United States, more than 75% of electricity generated is used to operate buildings. In China, rapid and widespread urbanization present prime opportunities to incorporate energy-efficient technologies and strategies into new buildings.

BEE research supports the development of innovations that will enable citizens to live and work in more comfortable, energy-efficient buildings. Essential technologies developed by this research will include:

- New, more energy-efficient and cost effective building insulation materials and cool roofs
- Enhanced ventilation and climate control technologies that improve indoor comfort and reduce energy consumption
- Buildings that integrate renewable (e.g., wind, geothermal, and solar) energy systems so that they generate more energy than they consume
- High-quality, energy-efficient lighting and window systems
- Tools that help building operators identify opportunities to improve system energy efficiency and save money

*The CERC Building Energy Efficiency (BEE) Consortium conducts R&D on building energy efficiency technologies and strategies in the United States and China. BEE researchers are working to improve efficiency in new and existing buildings, save energy, reduce greenhouse gas emissions, increase indoor comfort, and reduce stress on the electric grid. As new construction proceeds around the globe, collaborative BEE research efforts are helping to lock in the tremendous potential energy savings for the long term via a more efficient and low-carbon built infrastructure.*

BEE works to accelerate innovation leading to commercial successes that will improve the building design, building envelope, building equipment, whole building integration, and the monitoring and simulation of building energy consumption. As agreed upon by the U.S. and China consortia leaders, BEE has developed a strategy to achieve cost effective very low energy buildings (VLEBs) through a collaborative research agenda with 17 projects organized around the following topics (see Appendix F for more detail on BEE research activities):

- A. Integrated Building Design & Operation of Very Low Energy, Low Cost Buildings
- B. Building Envelope
- C. Building Equipment
- D. Renewable Energy Integration
- E. Whole Building
- F. Operation, Management, Market Promotion and Research

Illustrative technical highlights from across the BEE teams are discussed on the following pages.

## Significant BEE Joint Programmatic Activities in Year 2

Leadership from the BEE Consortium held three critical program planning, strategy setting, and review meetings:

- First CERC BEE Annual Review in Shenzhen, China, to assess previous year's activities
- Second CERC BEE Annual Review in Sanya, China, to agree on criteria for future project selection
- Joint Program Planning Meeting in Beijing to select continuing and new projects





# Key Achievements in Building Energy Efficiency

## Tools developed to facilitate integration of low-energy building systems and microgrids

Researchers at government laboratories, universities, and industry partners in the United States and China developed a cloud tool for the design of low-energy building systems and microgrids. It is currently being extended to optimize building control. This integrated approach could lower energy costs and carbon emissions by 30%, opening opportunities for vendors of controls, batteries, combined heat and power technologies, and other products. (Refer to page F20, Appendix F: BEE project number D/E2)



Microgrid testing and research have generated advancements in efforts to integrate distributed energy supply and optimize building control.

## Building energy modeling tools improved by integrating human behavior

CERC researchers studied human behavior in building energy systems and determined that the largest variable in building operating efficiency, compared to design, is the human factor. Based on these results, CERC researchers improved designer simulation tools DeST (Designer's Simulation Toolkit) and EnergyPlus to integrate human behavior into design calculations, potentially reducing energy use in new buildings up to 70% and pointing to opportunities for improved control systems in existing buildings.

Researchers developed new methods and simulation tools to quantify relative impact of human behavior on building energy performance. The tools and findings provide support for the development of effective energy codes and efficient building designs that can significantly reduce energy consumption. (Refer to page F5, Appendix F: BEE project number A2)



Improved tools that integrate human behavior into building design can reduce energy use in buildings, including new high rise buildings shown here in Shanghai.

## Cool roof simulations and demonstrations illustrate benefits under range of conditions

CERC researchers are developing improved white (cool) roof coatings with superior reflectance, durability, and self-cleaning properties for U.S. and Chinese markets. Energy use simulations quantified the benefits of these coatings in various settings and support the establishment of rating systems, incentives, and standards in China.

These simulations found that cool roofs saved energy and reduced CO<sub>2</sub> emissions in all Chinese climates with hot summers. A demonstration of cool roofs in a Chongqing, China, office building showed surface temperature reductions up to 20°C and daily electricity savings of about 9%. Research on new acrylic coatings for cool roofs can increase soiling and water resistance, energy savings, and durability. (Refer to page F13, Appendix F: BEE project number B3)

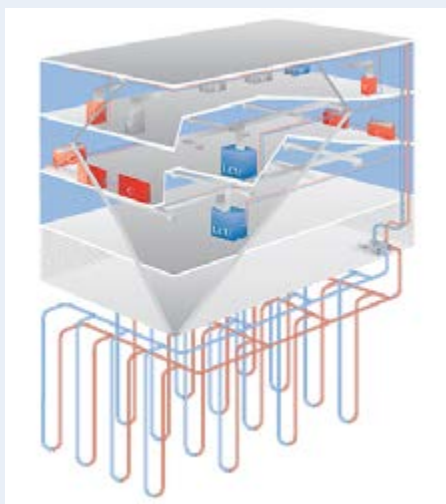


Research on white (cool) roof coatings is increasing cool roof performance, which facilitates greater market penetration that could result in significant energy savings.

# Key Achievements in Building Energy Efficiency

## Improved efficiency and cost of ground-source heat pumps

CERC researchers evaluated emerging ground-source heat pump (GSHP) technologies in both the United States and China, pointing to technology advancements in heat exchangers and improvements in GSHP efficiency and cost. Researchers identified alternative ground heat exchangers that require 21%–36% less drilling depth compared with conventional ground heat exchangers while retaining the same performance. By participating in demonstrations in the other's territory, this work also established a foundation for commercial cooperation in areas of mutual benefit. (Refer to page F16, Appendix F: BEE project number D2)



Emerging GSHP designs and technologies can reduce the cost and improve the performance of the systems.

## Commercial building energy use tool developed

A web-based benchmarking tool for hotels and commercial offices in China was completed by CERC researchers. The tool accounts for key drivers of energy use, including size, location, and operating hours, and incorporates data from hundreds of Chinese hotels and commercial offices. Researchers are comparing the findings from the tool to analogous properties in the United States. There are significant potential energy and CO<sub>2</sub> emission reductions identified by the tools, which can lead to market opportunities for green technology suppliers in both the United States and China. (Refer to page F7, Appendix F: BEE project number A3)



The hotel benchmarking tool is complete and available online at <http://www.cabr-cecc.com/>.

## Window shading attachments achieved significant energy savings

Researchers completed a technical assessment of the energy-savings potential of energy-efficiency measures that are likely to produce significant reductions in energy use in commercial buildings and published the findings in a journal article. Compared to the energy-efficiency code in effect in China, conventional low-emittance windows with exterior operable shading are able to achieve up to 66% savings in perimeter zone HVAC electricity consumption, 5% savings in district heating energy in the cold climate of Beijing, and up to 42% savings in HVAC electricity consumption in the hot/cold climate of Shanghai. Highly insulating windows also had a significant effect on reducing energy use. Shading attachments are likely to be a near-term, low-cost solution for retrofit and new construction in both the United States and China. (Refer to page F9, Appendix F: BEE project number B1)

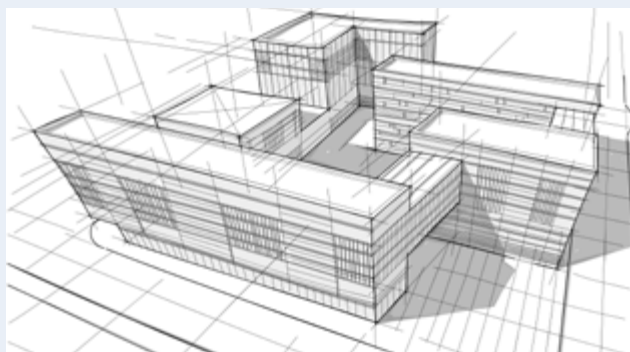


Rendering of the new addition to the Saint-Gobain Research Center in Shanghai where electrochromic windows will be evaluated in two side-by-side conference rooms.

# Key Achievements in Building Energy Efficiency

## Tailored software package improves use of natural ventilation in building design

CERC researchers developed an upgraded building design software tool that promotes the use of natural ventilation systems, which can increase energy efficiency and improve indoor climatic conditions. The software tool simulates ventilation fans and air conditioning units, predicting the effects on internal temperatures and airflow rates in buildings. Through a survey of natural ventilation applications in the United States and China, a lack of appropriate simulation programs was found to be an important factor that was inhibiting greater use of natural ventilation technologies. The building design software tool helps address this barrier. CERC researchers also analyzed different ventilation strategies to determine energy savings potential in ten climate zones from natural ventilation. (Refer to page F14, Appendix F: BEE project number B4)



Natural ventilation systems incorporated into building designs can increase energy efficiency and improve indoor comfort.

## Building Energy Efficiency (BEE) Partners

The U.S. BEE Consortium is led by **Lawrence Berkeley National Laboratory**. The U.S. Consortium includes the following partners:

- Bentley Systems Inc.
- C3 Energy
- ClimateMaster
- Dow Chemical Company
- The Energy Foundation, China Sustainable Energy Program
- ICF International
- Lutron Electronics
- Massachusetts Institute of Technology
- Natural Resources Defense Council
- Oak Ridge National Laboratory
- SAGE Electrochromics

The China BEE Consortium is led by the **Center of Science and Technology of Construction, Ministry of Housing and Urban-Rural Development (MOHURD)**. The China Consortium includes the following partners:

- |  |  |  |
|--|--|--|
| • Anhui Roba Energy Saving Technology Co.                  | • East-West Control Group (Shenyang) Co.               | • Equipment Company Co.  |
| • Beijing Ever Source Science & Technology Co.             | • ENN Group Co.  | • Shanghai Qingying Industrial Shares Co.  |
| • Beijing Huaqing Geothermal Development Co.               | • Guangzhou Zhengli General Electric Co.               | • Solatube CECIC Daylight Technology Co.   |
| • Beijing Huayi Leye Energy Service Co.                    | • Himin Solar Energy Group                             | • Telchina (Shandong) Co.  |
| • Beijing Lampower Photoelectric Co.                       | • Jiangsu Aide Solar Energy Technology Co.             | • Tianjin University   |
| • Beijing Persagy Energy Saving Technology Co.             | • Jiangsu Disimai GSHP Air Control Co.                 | • Tongguang Jaingong Construction Group Co.  |
| • Beijing Zhongchengke Green Building Technology           | • Jiangsu Refrigeration & Heating Saving Equipment Co. | • Tongji University  |
| • China Academy of Building Research                       | • Jiangxi Lattice Lighting Co.                         | • Tsinghua University  |
| • China Lanp Electrical Co.                                | • Jilin Kelong Building Energy-Saving Technology Co.   | • Wuxi Suntech Power Co.   |
| • Chint Solar (Zhejiang) Co.                               | • Landsea Group  | • Xinghua Green Industry International Low Carbon Technology Development (Beijing) Co. |
| • Chongqing University                                     | • LH Technology Co.                                    | • Xinjiang Green Refreshing Angel Environment Technology Co.                           |
| • Chongqing Zhonghai Industry Co.                          | • Liaoning Solar Energy R & D Co.                      | • Yingli Energy (Beijing) Co.  |
| • CISDI Engineering Co.                                    | • Nanjing Fullshare Energy Technology Co.              | • Zhejiang Dun'an Artificial Environmental Equipment Co.                               |
| • CSUS Green Lighting Science & Technology Research Center | • Nari Technology Development Co.                      | • Zhongji Yuanxiong Energy Storage Technology Co.                                      |
| • Dasheng Roller Shutters (Shanghai) Co.                   | • Shanghai Convertergy Energy Technology Co.           | • Zhuhai Singyes Green Building Technology Co.   |
| • Dongguan Vanke Building Technology Research Co.          | • Shanghai Fuka Construction & Engineering Co.         |  |
|  | • Shanghai Futian Air Conditioning                     |  |



# Clean Vehicles Consortium



## Vision of the Clean Vehicles Consortium

Contribute dramatic improvements in technologies to reduce the dependence of vehicles on oil and improve vehicle fuel efficiency in both countries. Perform long-range transformational and translational research to bring discoveries and technologies to market in the United States and China to advance technologies for clean vehicles.

## Collaborative Vehicles Research Generates Benefits in Both Countries

Clean vehicles research supports the development of innovations that will enable citizens to drive in safe, lightweight vehicles that use less fuel or use alternative fuels, such as electricity and biofuels. It will help deliver a range of essential technologies:

- Novel, efficient, and powerful battery designs for electric vehicles
- Tools to support the rapid design of powertrains for electric vehicles
- Monitoring devices to ensure the reliability, performance, and service life of electric vehicle batteries
- Tools to coordinate the charging of electric vehicles with power grid resource requirements
- Materials that recover and reuse energy lost as heat
- Advanced biofuels and new vehicle systems
- Processes for producing and joining lightweight materials that reduce vehicle weight and fuel use while ensuring strength and safety

*In 2012, sales of hybrid, plug-in, and pure electric vehicles (xEVs) in the United States increased from 287,000 units to 488,000 units. While this growth is impressive, xEVs captured only 3.4% of the light-duty vehicle market. Accelerating the pace of R&D could significantly reduce carbon emissions and other fossil fuel impacts in both the United States and China.*

The CERC Clean Vehicles Consortium (CVC) has collaboratively expanded basic research knowledge, technology development, and coordination between the two countries. The focus of CVC over the last year continues to be to (1) conduct high-quality research in identified key technology areas of clean vehicles, (2) promote and strengthen research collaborations between the United States and China, and (3) closely involve strategically targeted stakeholders, especially U.S. and Chinese companies, to encourage fast translation of the research and engineering work into commercial products. These efforts are advancing solutions to reduce the oil-dependence of vehicles and to improve vehicle fuel efficiency.

CVC projects have already resulted in 20 patents and invention disclosures in the United States, 12 patents in China, 152 published or accepted papers, and more than 100 personnel exchanges among participating organizations. CVC has developed a highly collaborative research agenda organized into six thrusts (see Appendix G for more details):

1. Advanced Batteries and Energy Conversion

## Major CVC Events Held in Year 2

The CVC was involved in several joint meetings in 2012-2013, including:

- Led the second CERC CVC Annual Review in Ann Arbor, U.S., to review previous year's activities, discuss partner participation, coordinate student exchanges, and plan for 2013
- Contributed to the EVI Symposia in Hangzhou, China, and Boston, U.S., to exchange information on electric vehicle deployment

2. Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
3. Vehicle Electrification
4. Lightweight Structures
5. Vehicle-Grid Integration
6. Energy Systems Analysis, Technology Roadmaps and Policies

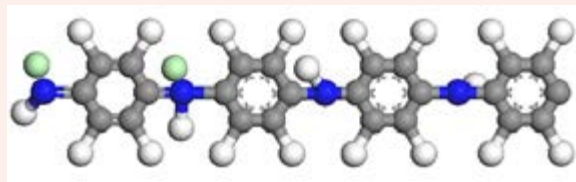
Highlights of CVC technical milestones in 2012-2013 are discussed on the following pages.

# Key Achievements in Clean Vehicles

## Novel cathode design for batteries shown to slow degradation and improve performance

Researchers examined nanomechanical properties that cause degradation in battery performance that are representative of actual driving conditions for electric vehicles (EVs), hybrid EVs (HEVs), and plug-in HEVs. By characterizing degradation and aging mechanisms of batteries, researchers are formulating design principles to improve battery cycle life. Researchers identified a polymerization mechanism that slows battery degradation.

Li-S batteries, which use a sulfur-based cathode, are a type of “beyond Li-ion” chemistry with the potential to exceed the energy density of today’s Li-ion batteries. The cycle life of these systems is limited due to the so-called “sulfur shuttle,” wherein soluble lithium polysulfides migrate from the cathode and damage the anode. CERC researchers demonstrated a new cathode design that minimizes this phenomenon by applying a polymer coating to encapsulate nanotube core/sulfur shell cathodes. This architecture slows degradation and improves performance while maintaining capacity. (Refer to page G4, Appendix G: CVC project number 1.1.1)



Polymerization creates a shell that prevents the sulfur shuttle mechanism, which causes battery degradation.

## Computationally efficient finite element tools developed that enable fast design iterations for lightweighting

CERC researchers simulated lightweight car body performance under crash safety tests by developing a model that uses complex and variable designs with many lightweight and other steel-substitute materials. The newly proposed methods were found to be dramatically faster than existing methods and are now being applied to search for improved EV motor designs. Experimental work in China is exploring substitution of amorphous iron for silicon steel laminations, which could enable higher efficiency and power density in electric machines. These findings provide essential input for predictive modeling tools used in conceptual lightweight vehicle crash analyses, enabling more efficient designs for lightweighting that improves vehicle fuel efficiency. (Refer to page G40, Appendix G: CVC project number 4.3.1)



Post-test specimens help characterize the failure mechanisms of crash analyses of high-strength steels.

## Materials sourcing and driving behavior study helps focus battery design for EVs

CERC researchers used GPS tracking software on 1,000 vehicles to reveal that 60% of Beijing drivers travel less than 25 miles per day. The 40-mile daily average for U.S. drivers had guided U.S. design criteria for battery-sizing of the Chevrolet Volt. Based on this information, General Motors could downsize the Volt’s battery in the Beijing market and still provide a level of service similar to that provided in the United States. Researchers simulated a Plug-in Hybrid Electric Vehicle similar to the Chevrolet Volt and examined the impact of vehicle component materials on lifecycle energy and emissions. Findings from the research are advancing development of an electrical grid model that includes renewable energy and lower carbon-based electricity strategies. (Refer to page G60, Appendix G: CVC project number 6.5)

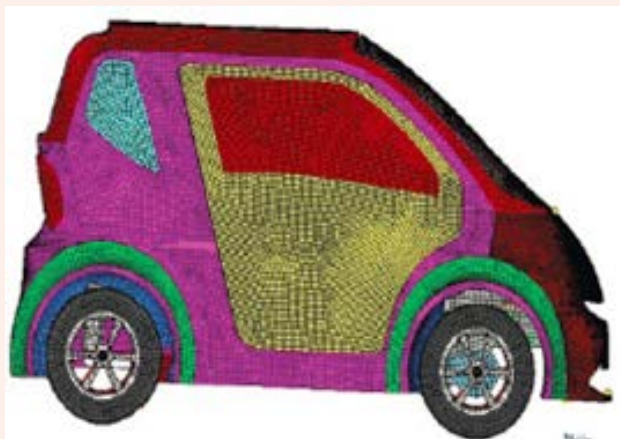


Characteristics of the Chevrolet Volt are included in a CERC-developed model that examines lifecycle impacts of vehicle component materials.

# Key Achievements in Clean Vehicles

## Modeling results utilized to optimize design of lightweight vehicle bodies

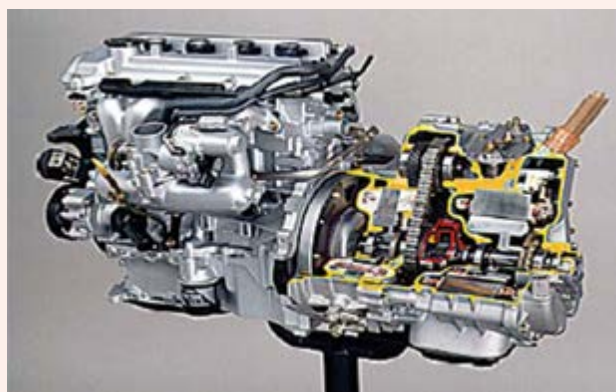
CERC researchers developed a model that simulates performance of vehicle bodies made of lightweight and other steel-substitute materials under crash safety tests. The model allows rapid exploration of thousands of variations in structural and geometric parameters for optimizing the safe and economical design of the lightweight bodies for clean powertrain vehicles. Researchers used computer-aided engineering models to study the effects of battery layouts on crashworthiness and to optimize its aerodynamic performance. (Refer to page G44, Appendix G: CVC project number 4.4)



Using computer-aided engineering models, researchers have been able to modify structural parameters for optimizing the design of lightweight vehicle bodies.

## Novel materials developed that facilitate conversion of waste heat to electricity

CERC researchers from the United States and China developed novel thermoelectric materials based on abundant, inexpensive compounds that, in their conduction form, achieved significant thermoelectric improvements. Efforts are underway to develop new forms of the material. Thermoelectric modules based on these compounds could significantly advance the efficient conversion of waste heat into electricity in internal combustion engine (ICE) vehicles. The research team has published six joint U.S.-China papers based on the project findings. (Refer to page G28, Appendix G: CVC project number 2.8)



Thermoelectric materials can produce electricity by utilizing waste heat from internal combustion engines, such as the one shown here.

## EV charging station simulations revealed potential benefits to electricity and transport systems

Researchers completed simulations of EV charging station location strategies, aiming to optimize coordination of the electricity and transport systems. Researchers found that common strategies today will burden the systems, and the research team proposed an alternate EV charging evaluation method that is more useful for evaluations of power systems with large-scale EV integration, including wind. The coordinated EV-wind simulations showed significant reductions in total system operation costs, wind curtailment, and emissions, and also a decrease in EV owners' charging fees. (Refer to page G46, Appendix G: CVC project number 5.1.1)



Locations of EV charging stations have been among the factors examined by CERC researchers to identify significant opportunities for improving coordination between road networks and electricity systems.



# Key Achievements in Clean Vehicles

## Clean Vehicle Consortium (CVC) Partners

The U.S. CVC is led by the **University of Michigan**. The U.S. consortium includes the following partners:

- Aramco Services
- Argonne National Laboratory
- Delphi
- Denso
- Eaton
- Environmental Protection Agency
- Ford Motor Company (Ford)
- Honda R&D Americas, Inc.
- Joint Bio Energy Institute
- Massachusetts Institute of Technology
- Oak Ridge National Laboratory, Energy and Transportation Science
- The Ohio State University
- PJM Interconnection
- Sandia National Laboratories, Combustion Research Facility
- TE Connectivity
- Toyota Motor Company, Toyota Motor Engineering and Manufacturing North America

The China CVC is led by **Tsinghua University**. The China consortium currently includes the following partners:

- Beihang University
- Beijing Institute of Technology
- Beijing Keypower
- Changzhou ECTEK Automotive Electronics Limited
- China Automotive Engineering Research Institute Co.
- China Automotive Technology & Research Center
- China Potevio
- Chinese Academy of Sciences
- Geely Group
- Hunan University
- JAC Motors
- Jingjin Electric Co.
- North China Electric Power University
- SAIC Motor
- Shanghai General Motors Wuling
- Shanghai Jiao Tong University
- Tianjin Lishen Battery Joint-stock Co.
- Tianjin University
- Tongji University
- Wanxiang
- Wuhan University of Technology



Dr. Andrew Brown, Vice President and Chief Technologist at Delphi, speaking with CERC leaders at the January 2013 Steering Committee Meeting in Washington, DC.

“The U.S.-China collaboration is a unique opportunity to better leverage technology development for future green vehicles. It also provides market and consumer insights, which will lead to more cost-effective and efficient solutions.”

Dr. Andrew Brown  
Vice President & Chief  
Technologist  
Delphi



U.S. CVC Director Dr. Hwei Peng (left), U.S. Secretary of Energy Dr. Steven Chu (center), and Eaton Chief Scientist Dr. Haoran Hu (right) at the January 2013 Steering Committee Meeting.

“CERC-CVC provides an excellent collaborative platform for international companies and universities to work together and tackle the common challenges we face in developing sustainable transportation solutions. As an active member of CERC-CVC, we are able to collaborate with customers, partners, and universities on key pre-competitive areas, which aligns well with Eaton’s open innovation strategy and commitment to developing clean energy technologies and products that meet the needs of our customers and benefit the environment.”

Dr. Haoran Hu  
Chief Scientist  
Eaton

# Intellectual Property Framework



## Protection of IP Promotes Innovation

Strong protection of IP encourages innovation in three ways:

- Encourages researchers to take risks and develop innovations confident that their intellectual property will be protected
- Allows others to access new knowledge through lawful means, promoting greater diffusion of technology
- Enables others to build on new discoveries, accelerating further innovation



“CERC creates a foundation for intellectual property protection and demonstrates the kinds of things that lie on this path of successful bilateral cooperation.”

Dr. Wan Gang  
Minister  
China Ministry of Science  
and Technology

*Protecting intellectual property (IP) is essential for developing technology innovations. A strong IP framework encourages bilateral cooperation among CERC researchers and instills confidence that their discoveries will be protected. The United States and China have launched an education and training program to help CERC researchers better understand the IP framework outlined in the Technology Management Plans (TMPs) and other pertinent IP laws and policies in each country.*

CERC's groundbreaking framework for protecting intellectual property supports and encourages joint research and innovation. The CERC Protocol, the U.S.-China CERC's founding document, features a novel and flexible Intellectual Property Annex, which strengthens IP protection and provides precedent-setting terms to foster joint creation and exchange of IP.<sup>1</sup> The framework is unique in that it gives each country a guaranteed right to exploit IP in the other country's territory, which can facilitate access to expanded markets for new technologies.

Three Technology Management Plans, jointly endorsed by the U.S. and Chinese governments, define the extent of that guaranteed right and outline other essential IP provisions (see sidebar on next page). All CERC research projects comport with the TMPs, which reflect fundamental IP principles in global commercial practice as well as in U.S. and Chinese law, and also include provisions for resolving disputes

consistent with international trade law (such as the United Nations Commission on International Trade Law).

By ensuring that IP will be protected, this framework encourages real joint collaboration. The competitive interests of partners are protected, which enables researchers to safely bring forward their best ideas and most innovative thinking. The U.S. and Chinese government endorsement of the framework and TMPs enables oversight and encourages compliance.

As a result, U.S. and Chinese teams are able to openly collaborate on and exchange information about research and development, which is accelerating progress and driving key technological breakthroughs. In addition, an increasing number of industry partners are joining CERC efforts, confident that their intellectual property will be protected and that they will be able to receive appropriate rewards for the innovations they create.

<sup>1</sup> The CERC Protocol and the IP Annex are available for download from the CERC website, <http://www.us-china-cerc.org/pdfs/protocol.pdf>

In the past year, CERC conducted a variety of activities to educate U.S. and Chinese partners about the CERC IP framework, as well as the laws and practices in each country that can impact IP rights. These activities provided essential resources for participants regarding IP issues that may arise in CERC projects and in CERC-related contract negotiations.

### *Intellectual Property Workshops*

Two joint workshops on IP for all CERC participants were held in 2012 and early 2013 to bring together researchers, practitioners and experts in U.S.-China IP law. The workshops helped Chinese and U.S. participants better understand the unique features and benefits of the CERC IP framework as well as the relevant laws and practices that can impact IP protection in each country. The workshops created a constructive environment and an ongoing dialogue that is helping new and existing participants to more fully engage in R&D collaboration and IP commercialization through CERC. The respectful and thoughtful tone of the workshops has fostered a greater collaborative spirit on both sides, driving increasingly forthright and useful discussions about IP issues and agreements.

The first CERC-wide IP workshop, held in Haikou, China, in March 2012, discussed CERC and its IP provisions and explored ways in which the United States and China can work together to strengthen IP protection and manage IP in joint research. The second CERC-wide IP workshop, held in Palo Alto, California, in February 2013, built on—and extended—the work of the

Haikou workshop. The second workshop covered issues related to IP in clean energy collaborations, with a special focus on differences in IP protection under Chinese and U.S. law.

The workshops also brought out some key lessons learned to date regarding collaboration and negotiation under the CERC IP framework and relevant laws and practices in each country. For example, the workshops highlighted key differences between U.S. and China law for patents, exclusivity, the protection of trade secrets, and the legal discovery process; the benefits and opportunities of conducting R&D under U.S.-China governmental agreements in general and the CERC IP arrangement in particular; and the ways that U.S. and Chinese IP laws (especially patent laws) are becoming more consistent. These kinds of insights are building a greater cultural and legal understanding that will help researchers in both countries to more easily and confidently enter into collaborative arrangements.

The workshops have been successful in providing a platform for knowledge exchange on key IP-related issues. Participants described the first workshop as groundbreaking, praising its open, bilateral nature and the breadth of material covered. The second workshop helped participants learn more specifically about how IP is treated in each country. Enthusiastic participation by attendees and a strong interest in continuing this program speak to the success of these workshops and the collaborative and trusting relationships it has been able to build between the two countries.

### **Joint Technology Management Plans central to novel IP Framework**

Technology Management Plans (TMPs) provide a foundation for protecting IP through CERC collaboration. CERC teams for each consortium negotiated separate TMPs, and these were endorsed by both the U.S. and Chinese governments.

Contrary to traditional partnership models where work plans are developed independently and there are minimal advantages to partners, the CERC's collaborative model takes on a completely new approach. CERC researchers jointly develop work plans, research is characterized by division of labor and shared results, and business partners are actively involved in the process from the beginning. The IP agreements have a common framework and are established before work begins.

This ground-breaking model provides an attractive platform for collaborative research and business investment because it protects the researchers and companies by assuring their rights to the IP and technologies they create. The model also dictates how intellectual property may be shared or licensed in each country. IP rights are guaranteed in each territory, and IP terms and conditions may be negotiated. When IP is created in a jointly funded research project, the project's participants in both countries have the right to obtain a non-exclusive license to the IP. The two governments oversee compliance and facilitate support. These features encourage openness and build confidence among researchers that their IP will be protected and that they will receive their due benefits.



Liu Yumin (left), President at GCL America, and Bill Jackson (second from left), Global R&D Director at Dow Chemical, moderated a panel of leading IP lawyers at the February 2013 IP workshop in Stanford, California: Dr. Yu Xiang (center), Professor at the Department of Technological Management and Intellectual Property at Huazhong University of Science and Technology; Dan Lang (second from right), Vice President for Intellectual Property at Cisco Systems; and Dr. Benjamin Bai (right), Partner at Allen & Overy.



## Key Findings from the CERC-wide IP Workshops

### Observations and Challenges

- Background IP is an important issue in collaborative R&D efforts and misunderstanding this term can damage relationships among parties.
- It is sometimes difficult to determine where an invention was completed, which can have implications on where a patent should be filed and the jurisdiction of national patent law. For an agreement to be enforceable in China, it must comply with mandatory provisions of Chinese law.
- Due to differences in IP rules and legal systems between the United States and China, misinterpretations of terms such as “exclusivity” and “technology transfer” can occur.
- China’s large number of individual patent inventors increases the risk of abusive patent litigation from non-practicing entities (“patent trolls”).
- Although U.S. programs aim to make patenting clean energy technologies easier and faster, there can still be substantial problems after the patent is issued in the form of excessive litigation or “patent thickets.”
- Trade secret protection is particularly challenging in the Chinese context due to a lack of mature legal protections for trade secrets.
- CERC can serve as a model in addressing IP more broadly in bilateral relations. Success of the CERC model can be partially attributed to a more flexible international IP regime than previous S&T agreements, while leaving room for additional details to be negotiated as needed by the CERC participants.

### Solutions and Recommendations

- U.S. and Chinese inventors would benefit from understanding the differences between the U.S. and Chinese patent systems.
- It is important to agree to the terms of an IP agreement prior to beginning work in order to avoid disputes, or at a minimum, having to reopen an agreement for negotiation.
- While negotiating under the TMP, both sides should clearly identify what each party can offer to the partnership at the outset, which can then form the basis for a legal agreement.
- It is critical to establish IP arrangements between parent firms in a joint venture (JV), which present unique IP protection concerns.
- Increased coordination between the U.S. and China patent offices is gradually increasing consistency between the two legal systems. A pilot program has been established to streamline the patent application process for inventors filing in both systems.
- Simple actions can prevent loss of trade secrets, such as disabling the use of USB drives and monitoring email attachments.

### Educational and Technical Resources

CERC provides an ongoing program of education and technical assistance throughout the year, creating valuable tools and resources that continue the learning and engagement sparked by the IP workshops. CERC experts in the practice of IP law in both countries collaborate on these important resources:

**The first “annotated” TMP.** Drafted by U.S. and Chinese CERC IP experts and presented at the Stanford IP Workshop, the annotated TMP explains the meaning or implications of certain provisions and how to implement these provisions of the TMP in specific projects. It will be a “living” document, revised as experience with the TMP grows.

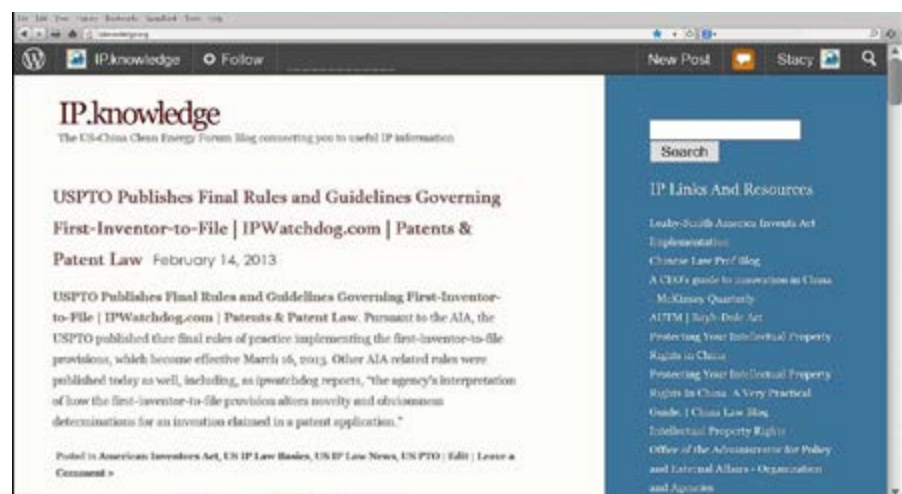
**The CERC IP Handbook.** Prominent U.S. and Chinese legal experts are drafting a guide that will elaborate IP and technology transfer law and strategies. The handbook will describe the law in easy-to-understand language and provide researchers and subject matter experts with a greater understanding of both U.S. and Chinese laws and practices in the context of CERC projects. The guide will focus on issues

that involve researchers or background intellectual property from both countries. The guide is “modeled” after the widely accepted handbook authored by the University of Michigan Technology Transfer Department.

**The IPknowledge.org web portal.** The regularly updated [www.ipknowledge.org](http://www.ipknowledge.org) portal connects CERC participants with

useful IP information and features a blog offering insight and commentary from leading experts.

**IP workshop presentations.** The bilingual presentations from the IP workshops, now available on the CERC website ([www.us-china-cerc.org](http://www.us-china-cerc.org)), offer valuable guidance and discuss some issues of greatest concern.



The U.S.-China Clean Energy Forum blog and website at [IPknowledge.org](http://IPknowledge.org) provides useful information, news, and opinions on intellectual property.



China CERC Director Counselor Liu Zhiming (left) and U.S. CERC Director Dr. Robert Marlay (right) at the IP workshop in Stanford, California, emphasized that successful collaboration between U.S. and China researchers has been facilitated by the novel CERC IP framework, which can also serve as a model for IP protection in future collaborations beyond clean energy in the future.

## Expanding Partnerships

In response to high interest among both industry and non-governmental organizations, DOE and MOST adopted a new agreement that provides a clear pathway and transparent, uniform process for new participants to join CERC's research consortia. The new procedures will be implemented immediately (see Appendix D for procedures for adding new members to the CERC consortia).

The agreement demonstrates CERC's commitment to unite the efforts of industry, academic researchers, and government experts to advance clean energy. Increased participation in CERC's research efforts can bring new ideas and perspectives that will drive innovation.



“While IP refers to ‘intellectual property,’ in the context of CERC it could also stand for ‘innovation promotion.’”

Dennis Bracy  
Chief Executive Officer  
U.S.-China Clean Energy Forum

## Intellectual Property Experts Working Group

The United States Department of Energy (DOE) and China Ministry of Science and Technology (MOST) established a new U.S.-China Intellectual Property Experts Group to identify and implement approaches to enhance innovation and the utilization, protection, and management of intellectual property for CERC. The group will also oversee IP education and technical assistance for CERC participants, developing solutions for approval by both governments that will be piloted in CERC projects.

The group will provide ongoing support to help participants better understand CERC's IP framework and key IP issues in U.S.-China collaboration. Ultimately, the group's work will enhance researchers' confidence in joint research, driving greater information exchange and innovation.

The group held its first meeting at Stanford Law School in February alongside the CERC IP workshop. Members are now starting to identify key issues that the working group will address.

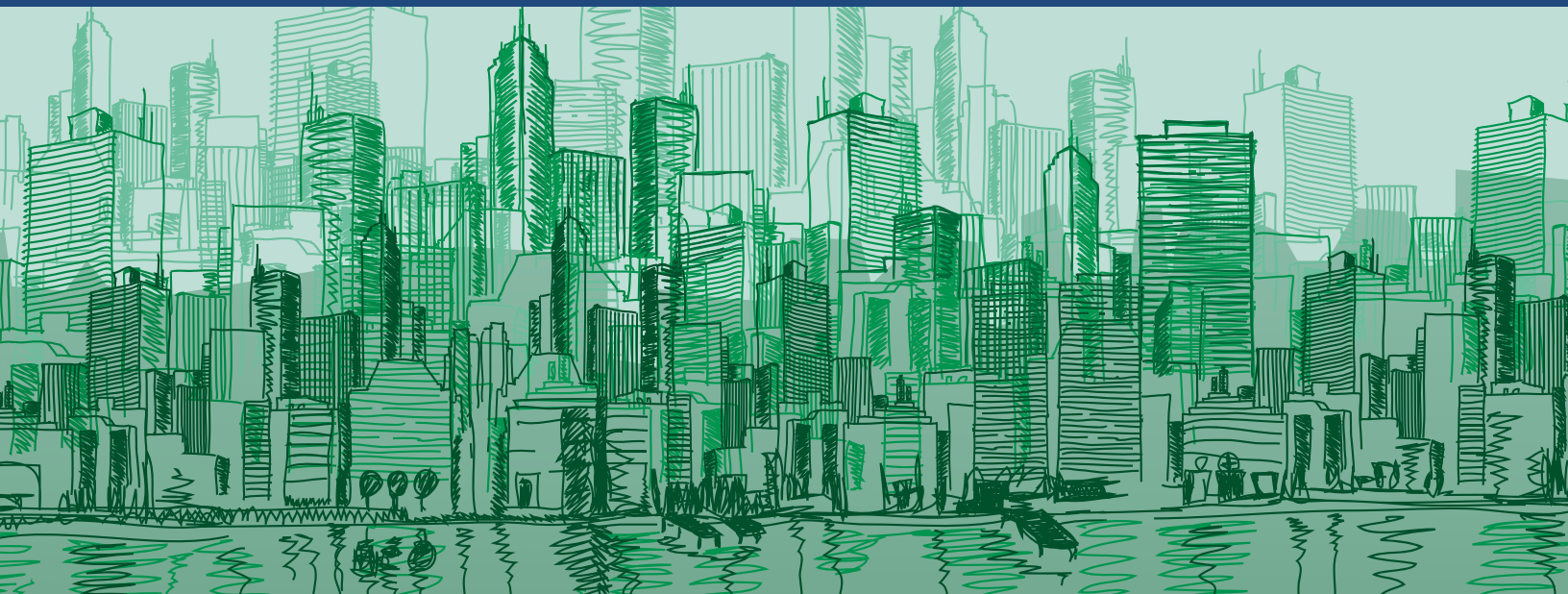


CERC's IP framework drives greater information sharing among researchers.



Researchers are sharing critical information to accelerate development of cleaner power generation, including integration of vehicles to the electric grid.

# Conclusions and Future Plans



“[New mechanisms for low-carbon growth in the United States and China] will translate then into opportunities for specific work around green technologies and research and development, and interactions between our scientists so that we can, together, help advance the goal of a sustainable planet, even as we continue to grow and develop.”

Barack Obama  
U.S. President

*Energy security, economic competitiveness, and environmental concerns arising from the production and use of energy remain pressing issues for the United States and China and will continue to be important for both countries for years to come. By accelerating research and development in the clean energy sector, CERC is answering the call for energy innovation at a critical juncture. Investments in CERC R&D are enabling the two countries to become frontrunners in the expanding global clean energy markets. CERC research teams have successfully built partnerships with industry, government, and others to spur innovation in clean technologies that are beneficial to both the United States and China.*

CERC made great strides in its second year of operation by further expanding and strengthening its collaborative program of R&D to advance clean energy in both countries. This visionary presidential initiative is working to accelerate development and deployment of critical clean energy technologies that will help diversify the energy supply, transition to a low-carbon infrastructure, and avoid the worst consequences of climate change. CERC has had impactful outcomes and substantive breakthroughs over the past year. With improved tools, designs, and demonstrations in areas such as co-generation power plants, CO<sub>2</sub> utilization with microalgae, cool roof coatings, building energy systems, Li-ion battery life, and vehicle-grid interactions, this

landmark initiative is successfully generating important clean energy technology advancements.

Business, government, and non-governmental entities are accruing benefits as a result of collaborations with research-performing organizations, and relationships between researchers and business partners at the working level are maturing. More than 100 businesses and non-governmental organizations are active participants, sharing industry experience and resources with CERC researchers and providing investments and in-kind contributions. In fact, growing interest by businesses and other stakeholders in clean energy research prompted CERC to publish a new process for adding potential partners to CERC's research consortia.



CERC's unique IP model has been a vital instrument in promoting innovative research and development. This model is embodied in the government-endorsed TMPs, which have proven to be a groundbreaking framework for bilateral S&T collaboration. The TMPs have also provided necessary structure for settling disputes over IP rights.

Four independent evaluations conducted in 2012 recognized CERC as an effective forum for pragmatic clean energy collaboration that clearly benefits both countries. The evaluations commended CERC's milestone IP initiative. Insights from the independent evaluations have enabled CERC to make targeted improvements, including the following: joint R&D planning processes have become more deliberate and the portfolios are being made more strategic; new selection criteria have been established for projects requiring joint participation by businesses in both countries; and only those projects that exhibit strong benefits for both countries and focus on technologies and innovations with the potential to create IP are being considered for inclusion in the CERC portfolio. The United States has also strengthened its management at CERC—leading institutions by hiring full-time operations managers to assist the technical leaders. CERC's revised research portfolio better aligns current activities with the initiative's broader strategic aims and also strengthens institutional ties with industry partners in both countries. Altogether, these improvements strengthen CERC and bolster its efforts in the development and rapid deployment of critical clean energy technologies.

### *Future Plans*

At the very heart of CERC, the three research consortia are achieving impressive technical breakthroughs. Cutting-edge research planned for the consortia includes the following:

**Advanced coal technology** research teams—having already developed new techniques, tools, and processes to reduce energy consumption, decrease costs, and reduce emissions—will collaborate to develop a better understanding of Chinese and U.S. best practices, evaluate these practices in selected Chinese plants, and summarize the results. R&D in 2013

will focus on techno-economic analysis, integrated gasification combined cycle (IGCC) systems, post-combustion CO<sub>2</sub> capture, criteria for new burner designs, oxycombustion technology on corner-fired boilers, and use of algae for the chemical capture of CO<sub>2</sub>. Finally, ACTC will focus on enhancing collaboration on research and academic exchanges between Chinese and American partners and on comparing best practices, conducting workshops, and further investigating improvements in advanced power generation technologies.

**Building energy efficiency** teams—having already improved climate control systems, building envelope materials, standards, and tools—will continue work to improve monitoring and simulation, building envelope, whole buildings, equipment, renewable energy, and related policies, and to strengthen engagement with Chinese business partners, find mutually beneficial opportunities to capitalize on a number of advanced building demonstrations, and facilitate U.S. business engagement. Critically, each demonstration would have a Research Development Test and Evaluation (RDT&E) component. Other areas of focus include the development of an online benchmarking tool; expanded use of real-time monitoring data; new designs for fenestration materials and systems; high-efficiency shading and insulated window systems; integrated control strategies; lighting demonstration programs; and policy recommendations for promoting energy efficiency, renewable energy, and green buildings.

**Clean vehicles** teams—which have provided new cathode designs, new materials, and improved simulation tools—plan to further enhance battery performance and inform battery and vehicle body design. Modeling efforts will improve understanding of the degradation of Li-ion batteries and facilitate design of processes to slow degradation. Research will also identify critical factors for battery energy and power capabilities, best practices for the placement of charging stations, and decentralized charging strategies. The models and concepts developed will reflect life-cycle, rather than just use-cycle, emissions to inform future fuel economy and greenhouse gas (GHG) standards.



“CERC is the most successful China-U.S. energy cooperation program since normalization of relations in 1979.”

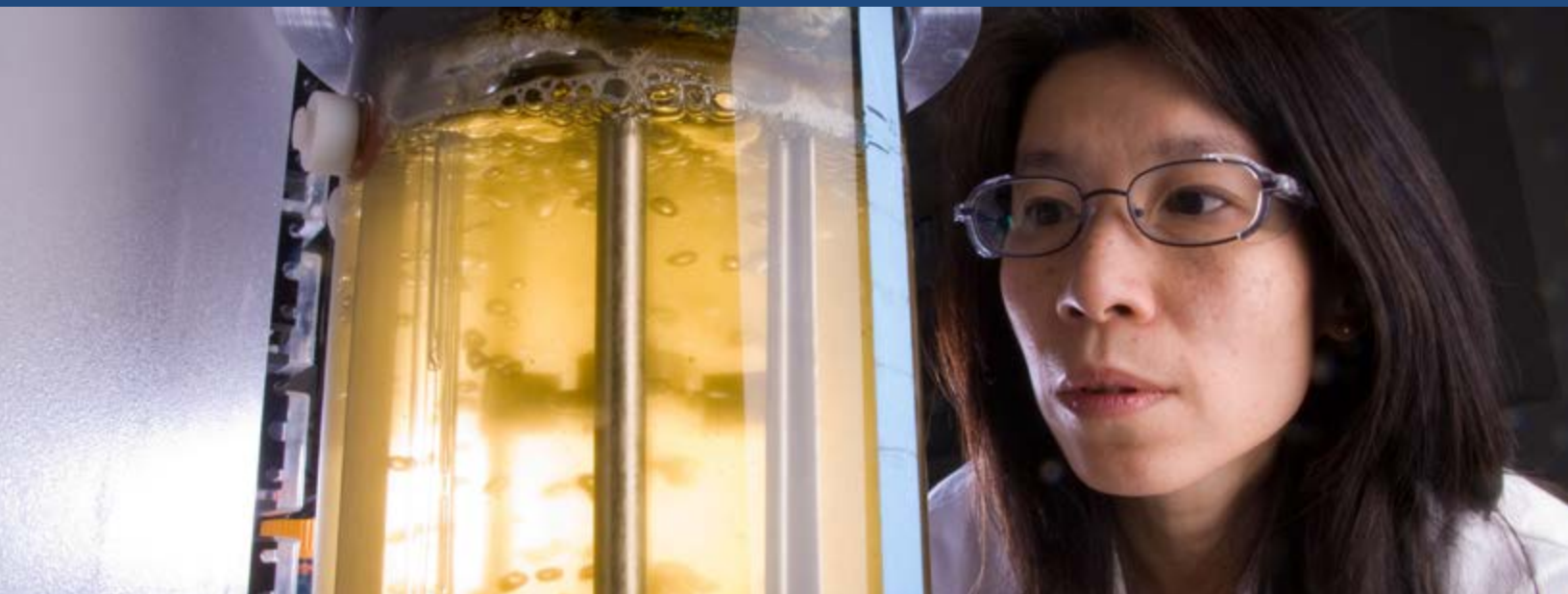
Dr. Jin Xiaoming  
Director-General  
International Department  
China Ministry of Science  
and Technology

**IP framework**—the pivotal enabler for this technical cooperation and achievement—will continue to be a focus of education, outreach, and technical support in 2013 and beyond. Both the United States and China will advance collaboration through the CERC IP Experts' Working Group, whose efforts will enhance IP protection and provide sufficient technical support to enhance understanding of IP issues and continued progress in joint U.S.-China research.

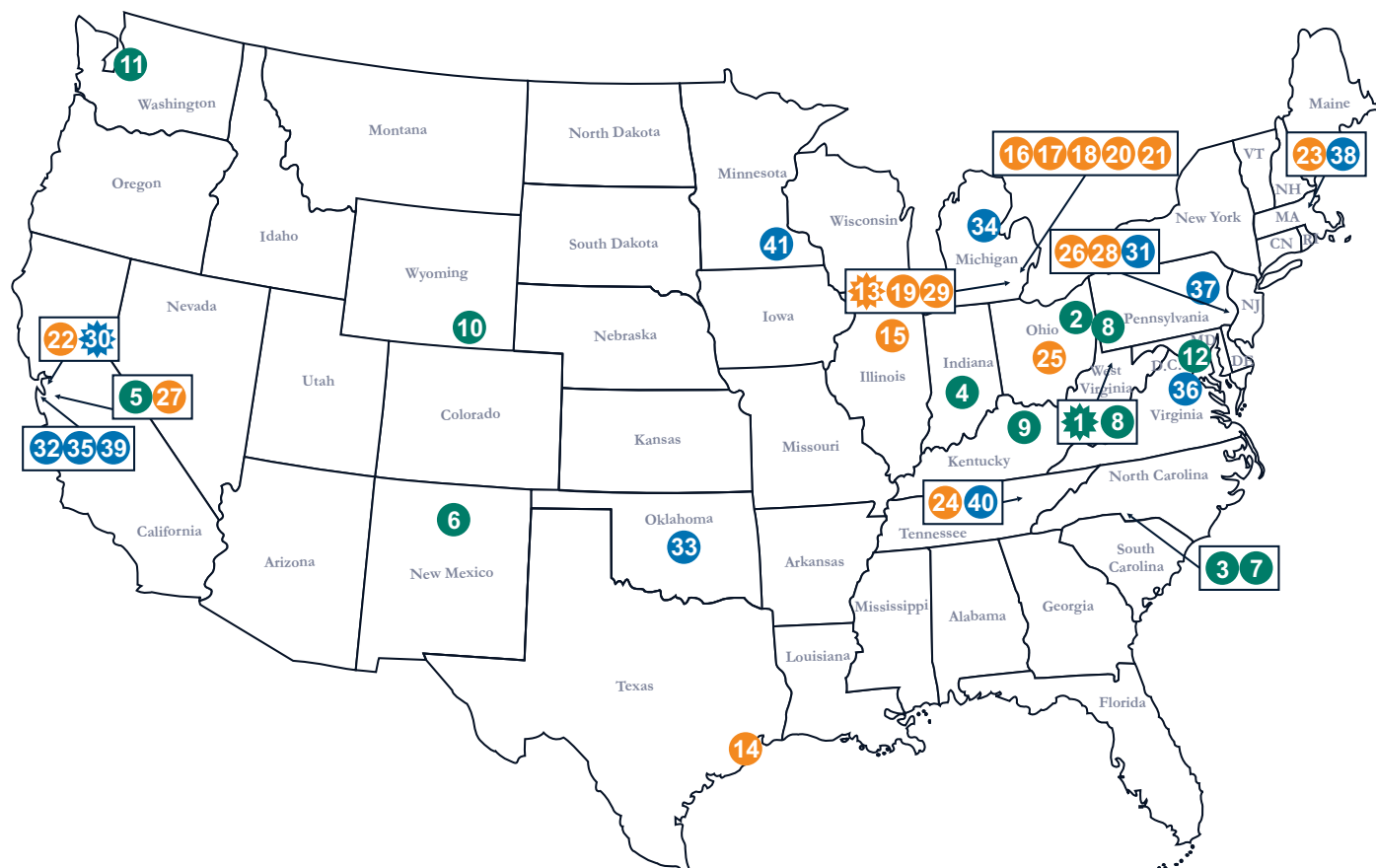
CERC provides a novel, exciting pathway for solving bilateral energy challenges more quickly, affordably, and expertly than each country could achieve working alone. In the near term, CERC is helping the United States and China leverage research and achieve important technical breakthroughs; accelerate technology deployment; and boost clean energy technology manufacturing, sales, and installation, both domestically and internationally. In the long term, CERC can help the United States and China realize the energy, economic, and environmental benefits of greater clean energy deployment, including greater efficiency, reduced energy use and costs, reduced pollution, mitigation of GHG emissions, and expanded markets for domestic businesses and industries.

CERC is predicated on the concept of a more flexible and ambitious model for bilateral science and technology cooperation. With continued strong support and encouragement from both governments, it will continue to enable and encourage collaboration by researchers on both sides to solve today's most pressing energy challenges.

# Appendices



# Appendix A: Maps of Consortia Partner Locations





## ACTC

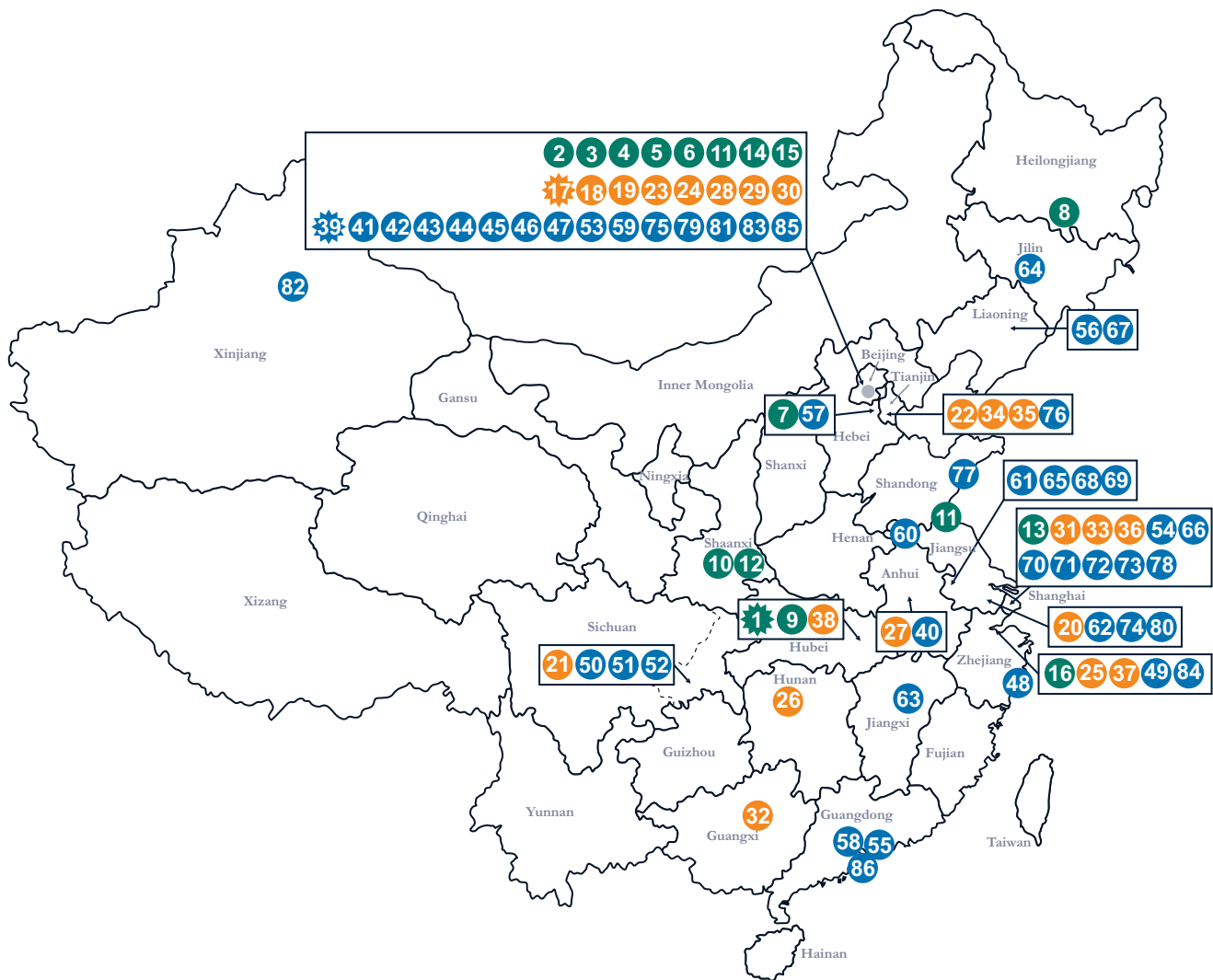
<b>1</b>	West Virginia University	Morgantown, WV
<b>2</b>	Babcock & Wilcox	Barberton, OH
<b>3</b>	Duke Energy	Charlotte, NC
<b>4</b>	Indiana Geological Survey	Bloomington, IN
<b>5</b>	Lawrence Livermore National Laboratory	Livermore, CA
<b>6</b>	Los Alamos National Laboratory	Los Alamos, NM
<b>7</b>	LP Amina	Charlotte, NC
<b>8</b>	National Energy Technology Laboratory	Morgantown, WV & Pittsburgh, PA
<b>9</b>	University of Kentucky	Lexington, KY
<b>10</b>	University of Wyoming	Laramie, WY
<b>11</b>	U.S.-China Clean Energy Forum, China Relations Council	Seattle, WA
<b>12</b>	World Resources Institute	Washington, DC

## CVC

<b>13</b>	University of Michigan	Ann Arbor, MI
<b>14</b>	Aramco Services	Houston, TX
<b>15</b>	Argonne National Laboratory	Argonne, IL
<b>16</b>	Delphi	Troy, MI
<b>17</b>	Denso	Southfield, MI
<b>18</b>	Eaton	Southfield, MI
<b>19</b>	Environmental Protection Agency	Ann Arbor, MI
<b>20</b>	Ford Motor Company	Dearborn, MI
<b>21</b>	Honda R&D Americas, Inc.	Southfield, MI
<b>22</b>	Joint Bio Energy Institute	Berkeley, CA
<b>23</b>	Massachusetts Institute of Technology	Cambridge, MA
<b>24</b>	Oak Ridge National Laboratory	Oak Ridge, TN
<b>25</b>	The Ohio State University	Columbus, OH
<b>26</b>	PJM Interconnection	Norristown, PA
<b>27</b>	Sandia National Laboratories, Combustion Research Facility	Livermore, CA
<b>28</b>	TE Connectivity	Berwyn, PA
<b>29</b>	Toyota Motor Company, Toyota Motor Engineering and Manufacturing North America	Ann Arbor, MI

## BEE

30	Lawrence Berkeley National Laboratory	Berkeley, CA
31	Bentley Systems Incorporated	Exton, PA
32	C3 Energy	San Mateo, CA
33	ClimateMaster	Oklahoma City, OK
34	Dow Chemical Company	Midland, MI
35	Energy Foundation, China Sustainable Energy Program	San Francisco, CA
36	ICF International	Fairfax, VA
37	Lutron Electronics	Coopersburg, PA
38	Massachusetts Institute of Technology	Cambridge, MA
39	Natural Resources Defense Council	San Francisco, CA
40	Oak Ridge National Laboratory	Oak Ridge, TN
41	SAGE Electrochromics	Faribault, MN





## ACTC

<b>1</b>	Huazhong University of Science and Technology	Wuhan
<b>2</b>	China Huaneng Group Clean Energy Research Institute	Beijing
<b>3</b>	China Huaneng Group Power International, Inc.	Beijing
<b>4</b>	China Power Engineering Consulting Group Corporation (CPECC)	Beijing
<b>5</b>	China Power Investment Corporation	Beijing
<b>6</b>	China University of Mining and Technology	Beijing
<b>7</b>	ENN (XinAo Group)	Langfang, Hebei
<b>8</b>	Harbin Institute of Technology	Harbin
<b>9</b>	Institute of Rock and Soil Mechanics, Chinese Academy of Science	Wuhan
<b>10</b>	Northwest University	Shaanxi
<b>11</b>	Research Center for Energy and Power, Chinese Academy of Sciences	Beijing & Lianyungang, Jiangsu
<b>12</b>	Shaanxi Yanchang Petroleum (Group) Co., LTD	Shaanxi
<b>13</b>	Shanghai JiaoTong University	Shanghai
<b>14</b>	Shenhua Group Corporation LTD.	Beijing
<b>15</b>	Tsinghua University	Beijing
<b>16</b>	Zhejiang University	Zhejiang

## CVC

<b>17</b>	Tsinghua University	Beijing
<b>18</b>	Beihang University	Beijing
<b>19</b>	Beijing Institute of Technology	Beijing
<b>20</b>	Changzhou ECTEK Automotive Electronics Limited	Changzhou, Jiangsu
<b>21</b>	China Automotive Engineering Research Institute Co., Ltd	Chongqing
<b>22</b>	China Automotive Technology & Research Center	Tianjin
<b>23</b>	China Potevio	Beijing
<b>24</b>	Chinese Academy of Sciences	Beijing
<b>25</b>	Geely Group	Hangzhou, Zhejiang
<b>26</b>	Hunan University	Hunan
<b>27</b>	JAC Motors	Hefei, Anhui
<b>28</b>	Jingjin Electric Co., Ltd	Beijing
<b>29</b>	Keypower	Beijing
<b>30</b>	North China Electric Power University	Beijing
<b>31</b>	SAIC Motor	Shanghai
<b>32</b>	Shanghai General Motor Muling	Liuzhou, Guangxi
<b>33</b>	Shanghai Jiao Tong University	Shanghai
<b>34</b>	Tianjin Lishen Battery Joint-Stock Co., LTD.	Tianjin
<b>35</b>	Tianjin University	Tianjin
<b>36</b>	Tongji University	Shanghai
<b>37</b>	Wanxiang	Hangzhou, Zhejiang
<b>38</b>	Wuhan University of Technology	Wuhan

## BEE

39	Center of Science and Technology of Construction, Ministry of Housing and Urban-Rural Development	Beijing
40	Anhui Roba Energy Saving Technology Co., Ltd.	Hefei, Anhui
41	Beijing Ever Source Science & Technology Development Co., Ltd.	Beijing
42	Beijing Huaqing Geothermal Development Co., Ltd.	Beijing
43	Beijing Huayi Leye Energy Service Co., Ltd.	Beijing
44	Beijing Lampower Photoelectric Co., Ltd.	Beijing
45	Beijing Persagy Energy Saving Technology Co., Ltd.	Beijing
46	Beijing Zhongchengke Green Building Technology Co., Ltd.	Beijing
47	China Academy of Building Research	Beijing
48	China Lanp Electrical Co., Ltd.	Leqing, Zhejiang
49	Chint Solar (Zhejiang) Co., Ltd.	Hangzhou, Zhejiang
50	Chongqing University	Chongqing
51	Chongqing Zhonghai Industry Co., Ltd.	Chongqing
52	CISDI Engineering Co., Ltd.	Chongqing
53	CSUS Green Lighting Science & Technology Research Center	Beijing
54	Dasheng Roller Shutters (Shanghai) Co., Ltd.	Shanghai
55	Dongguan Vanke Building Technology Research Co., Ltd.	Dongguan, Guangdong
56	East-West Control Group (Shenyang) Co., Ltd.	Shenyang, Liaoning
57	ENN	Langfang, Hebei
58	Guangzhou Zhengli General Electric Co., Ltd.	Guangzhou, Guangdong
59	Himin Solar Energy Group	Beijing
60	Jiangsu Aide Solar Energy Technology Co., Ltd.	Xuzhou, Jiangsu
61	Jiangsu Disimai Ground Source Heat Pump Air Control Co., Ltd.	Nanjing, Jiangsu
62	Jiangsu Refrigeration & Heating Saving Equipment Co., Ltd.	Peizhou, Jiangsu
63	Jiangxi Lattice Lighting Co., Ltd.	Nanchang, Jiangxi
64	Jilin Kelong Building Energy-Saving Technology Co., Ltd.	Changchun, Jilin
65	Landsea Group	Nanjing, Jiangsu
66	LH Technology Co., Ltd.	Shanghai
67	Liaoning Solar Energy R & D Co., Ltd.	Shenyang, Liaoning
68	Nanjing Fullshare Energy Technology Co., Ltd.	Nanjing, Jiangsu
69	Nari Technology Development Co., Ltd.	Nanjing, Jiangsu
70	Shanghai Convertergy Energy Technology Co., Ltd.	Shanghai
71	Shanghai Fuka Construction & Engineering Co., Ltd.	Shanghai
72	Shanghai Futian Air Conditioning Equipment Co., Ltd.	Shanghai
73	Shanghai Qingying Industrial Shares Co., Ltd.	Shanghai
74	Solatube CECIC Daylight Technology Co., Ltd.	Suzhou, Jiangsu
75	TelChina (Shandong) Co., Ltd.	Beijing
76	Tianjin University	Tianjin
77	Tongguang Jiangong Group Co., Ltd.	Qingdao, Shandong
78	Tongji University	Shanghai
79	Tsinghua University	Beijing
80	Wuxi Suntech Power Co., Ltd.	Wuxi, Jiangsu
81	Xinghua Green Industry International Low Carbon Technology Development (Beijing) Co., Ltd.	Beijing
82	Xinjiang Green Refreshing Angel Environment Technology Co., Ltd.	Urumqi, Xinjiang
83	Yingli Energy (Beijing) Co., Ltd.	Beijing
84	Zhejiang Dun'an Artificial Environmental Equipment Co., Ltd.	Hangzhou, Zhejiang
85	Zhongji Yuanxiong Energy Storage Technology Co., Ltd.	Beijing
86	Zhuhai Singyes Green Building Technology Co., Ltd.	Zhuhai, Guangdong

# Appendix B: CERC Organizational Structure

*The organizational framework of CERC leadership teams is built to facilitate bilateral cooperation that encourages interaction and ensures that both countries benefit from collective research.*

## CERC Governance

The CERC governance structure is headed by a Steering Committee composed of Ministers from the United States and China. The U.S. and China Secretariats report directly to their respective country's Steering Committee members, and are headed by government officials.

### *Steering Committee Members*

- U.S. Department of Energy Secretary, Dr. Ernest Moniz
- Minister of Science and Technology, Dr. Wan Gang
- National Energy Administrator, Dr. Wu Xinxiang
- (Ex-officio) Vice Minister of Housing and Urban-Rural Development, Dr. Qiu Baoxing

### *U.S. Secretariat*

- U.S. Department of Energy Acting Assistant Secretary for Policy and International Affairs, Jonathan Elkind
- U.S. CERC Director, Dr. Robert C. Marlay
- Director of East Asian Affairs, Dr. Casey Delhotal

### *Chinese Secretariat*

- Vice Minister, Cao Jianlin, Ministry of Science and Technology
  - Deputy Director General, Ma Linying, Ministry of Science and Technology
  - Chief Economist, Li Ye, National Energy Administration
  - Deputy Director General, Han Aixing, Ministry of Housing and Urban-Rural Development
- China CERC Director, Counselor Liu Zhiming, Ministry of Science and Technology
- Director, Americas and Oceania, Wang Qiang, Ministry of Science and Technology

Executive Committees for each of the three consortia report to the CERC Secretariat. These committees are composed of technical leaders and experts in the fields, and have up to five members each from the U.S. and China. The Executive Committees are tasked to provide oversight and to review CERC progress, to advise on the CERC portfolio and projects, and to identify opportunities for synergies with other related R&D programs.



# ACTC Executive Committee and Research Leadership

## *Executive Committee for Advanced Coal Technology*

- U.S. Committee Members
  - Chris Smith, Acting Assistant Secretary, for Fossil Energy, U.S. Department of Energy
  - Jarad Daniels, Director, Office of Clean Coal, U.S. Department of Energy
  - Dr. Darren Mollot, Director, Office of Clean Energy Systems, U.S. Department of Energy
  - Dr. Jay Braitsch, Senior Advisor for Strategic Planning, U.S. Department of Energy
- Samuel Tam, General Supervisory Engineer, Coal R&D Programs, U.S. Department of Energy
- Scott Smouse, Technology Manager, Advanced Combustion Systems, National Energy Technology Laboratory, U.S. Department of Energy
- Chinese Committee Members
  - Xiu Binglin, Deputy Director General of Department of Energy Conservation and Science & Technology Equipment, National Energy Administration
  - Zhou Dadi, Vice Chairman, China Energy Association
  - He Jiankun, Deputy Director, State Climate Change Expert Committee
  - Jiang Hongde, CAE Academician, Tsinghua University
  - Huang Qili, CAE Academician, Engineer-in-chief, Northeast China Grid Company

U.S. Research Management Team	China Research Management Team
Dr. Jerald J. Fletcher Director West Virginia University	Dr. Zheng Chugang Director Huazhong University of Science and Technology
Dr. S. Julio Friedmann Technical Program Manager Lawrence Livermore National Laboratory	Dr. Xu Shisen Chief Engineer Huaneng Clean Energy Research Institute
Dr. Qingyun Sun Collaboration Manager West Virginia University	Dr. Yao Qiang Chief Scientist Tsinghua University
Sam Taylor Operations Manager West Virginia University	

# BEE Executive Committee and Research Leadership

## *Executive Committee for Energy Efficient Buildings*

- U.S. Committee Members
  - Roland Risser, Deputy Assistant Secretary for Building Technologies, U.S. Department of Energy
  - Patrick Hughes, Director, Building Technologies Research and Integration Center, Oak Ridge National Lab
  - Dr. Hunter Fannery, Chief, Supervisory Mechanical Engineer, Building Environment Division, National Institute of Standards and Technology
- Richard Karney, Senior Technical Advisor, Emerging Technologies Team, Building Technologies, U.S. Department of Energy
- Chinese Committee Members
  - Tong Guichan, Director, Division of International Science & Technology Cooperation, Department of Building Energy Efficiency and Science & Technology, Ministry of Housing and Urban-Rural Development
  - Li Baizhan, Professor, Chongqing University
  - Xu Wei, Director, Institute of Building Environment and Energy Efficiency, China Academy of Building Research
  - Tan Hongwei, Professor, Tongji University
  - Zhu Neng, Professor, Tianjin University
  - Hao Bin, Director, Division of Industry Development, Center of Building Energy Efficiency, Ministry of Housing and Urban-Rural Development

U.S. Research Management Team	China Research Management Team
Dr. Nan Zhou Director Lawrence Berkeley National Laboratory	Liang Junqiang Director Science and Technology Center, Ministry of Housing and Urban-Rural Development
Dr. Yuan Yao China Liaison Lawrence Berkeley National Laboratory	Dr. Jiang Yi Technical Director Tsinghua University
Dr. Mark D. Levine Founding Director and Advisor Lawrence Berkeley National Laboratory	Wang Youwei Deputy Director Chinese Society for Urban Studies
Brian Heimberg Operations Manager Lawrence Berkeley National Laboratory	Liu Younong Program Manager Science and Technology Center, Ministry of Housing and Urban-Rural Development

# CVC Executive Committee and Research Leadership

## *Executive Committee for Clean Vehicles*

- U. S. Committee Members
  - Patrick Davis, Manager, Vehicles Technology Program, U.S. Department of Energy
  - Steve Goguen, Supervisor, Fuels, Combustion, & Deployment, U.S. Department of Energy
  - Dr. Larry Johnson, Director, Transportation Technology R&D Center, Argonne National Laboratory
  - Dave Howell, Team Leader for Hybrid and Electric Systems, U.S. Department of Energy
- Gurpreet Singh, Team Leader for Advanced Combustion Engine Technologies, U.S. Department of Energy
- Chinese Committee Members
  - Chen Jiachang, Deputy Director General, Department of High and New Tech, Ministry of Science and Technology
  - Zhang Jinhua, Deputy Secretary-General, Society of Automotive Engineers of China
  - Ren Xiaochang, Director, China Automotive Engineering Research Institute (CAERI)
  - Wu Zhixin, Deputy Director, China Automotive Technology & Research Center (CATARC)
  - Wang Binggang, China Society of Automotive Engineering
  - Wang Jiqiang, Deputy Chief Engineer, Tianjin Institute of Power Source

U.S. Research Management Team	China Research Management Team
Dr. Hwei Peng Director and China Liaison University of Michigan	Dr. Ouyang Minggao Director Tsinghua University
Dr. Jun Ni Deputy Director and China Liaison University of Michigan	Dr. Wang Hewu Deputy Director Tsinghua University
Carrie Morton Operations Manager University of Michigan	Dr. Qiu Xinping Deputy Director Tsinghua University



# Appendix C: CERC Funding

## Multi-Year Bi-Lateral CERC Funding Plan

Funding Fiscal Year <sup>1</sup>	Research Year <sup>2</sup>	Technical Track	United States		China	Consortium
			DOE	Partners	MOST & Partners	Totals
FY 2010	Year 0	Advanced Coal	\$2.5	\$2.7	\$0.0	\$5.2
		Buildings	\$2.5	\$0.0	\$0.0	\$2.5
		Clean Vehicles	\$2.5	\$1.1	\$0.0	\$3.6
		2010 Sub-Total	\$7.5	\$3.8	\$0.0	\$11.3
FY 2011	Year 1	Advanced Coal	\$2.5	\$2.7	\$4.6	\$9.8
		Buildings	\$2.5	\$2.8	\$3.5	\$8.8
		Clean Vehicles	\$2.5	\$3.2	\$4.4	\$10.1
		2011 Sub-Total	\$7.5	\$8.7	\$12.5	\$28.7
FY 2012	Year 2	Advanced Coal	\$2.5	\$3.2	\$9.2	\$14.9
		Buildings	\$2.5	\$3.2	\$8.9	\$14.6
		Clean Vehicles	\$0.0	\$3.0	\$4.2	\$7.2
		2012 Sub-Total	\$5.0	\$9.4	\$22.3	\$36.7
FY 2013	Year 3	Advanced Coal	\$2.5	\$2.7	\$5.0	\$10.2
		Buildings	\$2.5	\$4.0	\$5.0	\$11.5
		Clean Vehicles	\$3.4	\$3.0	\$5.0	\$11.4
		2013 Sub-Total	\$8.4	\$9.7	\$15.0	\$33.1
FY 2014	Year 4	Advanced Coal	\$2.5	\$2.7	\$5.0	\$10.2
		Buildings	\$2.5	\$2.5	\$5.0	\$10.0
		Clean Vehicles	\$2.5	\$3.0	\$5.0	\$10.5
		2014 Sub-Total	\$7.5	\$8.2	\$15.0	\$30.7
FY 2015	Year 5	Advanced Coal	\$0.0	\$0.0	\$5.0	\$5.0
		Buildings	\$0.0	\$2.5	\$5.0	\$7.5
		Clean Vehicles	\$1.6	\$0.0	\$5.0	\$6.6
		2015 Sub-Total	\$1.6	\$2.5	\$15.0	\$19.1
Multi-Yr Totals		Advanced Coal	\$12.5	\$14.0	\$28.8	\$55.3
		Buildings	\$12.5	\$15.0	\$27.4	\$54.9
		Clean Vehicles	\$12.5	\$13.3	\$23.6	\$49.4
		TOTAL	\$37.5	>\$37.5	>\$75.0	>\$150.0

Funded	Planned
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<sup>1</sup> Ending September 30<sup>th</sup>

<sup>2</sup> Ending December 31<sup>st</sup>

# Appendix D: Procedures for Adding New Members

March 29, 2013

## PROCEDURES FOR ADDING NEW MEMBERS TO CONSORTIA FOR THE CLEAN ENERGY RESEARCH CENTER

Business, industrial, and non-governmental entities that have been contributing to and collaborating with research-performing organizations operating under the auspices of the U.S.-China Clean Energy Research Center (CERC) are seeing results and accruing benefits from CERC participation.<sup>1</sup> As a consequence of these early successes, other research institutions and businesses in both countries have expressed interest in joining CERC consortia as new members and participating in CERC cooperative activities.

The U.S. Department of Energy, and the Ministry of Science and Technology and the National Energy Administration of the People's Republic of China, have reached the following understanding:

1. In general, enhanced engagement by business, industrial, and non-governmental entities in CERC cooperative activities, through greater participation and by adding new consortia members, is encouraged. A new CERC consortium member is expected to:
  - (a) Support the mission of the CERC as established by the Protocol and the vision and goals of its respective CERC consortium as established by the consortium director
  - (b) Add value to the CERC's capacities and work program, evidenced in part by contributions of an intellectual, technical, financial, and/or in-kind nature
  - (c) Support projects that meet CERC criteria<sup>2</sup>
  - (d) Agree in writing to be bound by the same obligations of an existing consortium's members; and
  - (e) Agree in writing to adhere to the provisions of the Protocol and the associated Technology Management Plans governing the protection and allocation of intellectual property arising from CERC cooperative activities.<sup>3</sup>
2. In order to assure that new consortium members adhere to the CERC mission and meet the standards set by the Protocol's signatories, the following procedures are to apply to the addition of new consortium members:
  - (a) An interested entity and prospective member should submit a formal request to join a U.S. or China CERC consortium to that country's consortium director.
  - (b) The request should provide a description of the entity and any other relevant information (e.g., a brief description of projects it is interested in undertaking in the CERC, potential project partnerships with existing consortium members, and the nature of the contribution(s), of the type stated in paragraph 1(b) above, it may be willing to make to the CERC.
  - (c) A request should include a letter signed by an authorized official of the applying entity stating the applicant's commitment to be bound by the Technology Management Plan for the relevant consortium.
  - (d) Upon receipt of the request, and after consultation with other consortium members, the CERC consortium director receiving the request is to consult with the other country's consortium's director.
  - (e) After such consultation and consideration of views, the consortium director, alone, shall determine whether the request conforms to the requirements above and membership be granted.
  - (f) If granted, the consortium director shall inform the CERC Secretariat.
3. Each country consortium director shall maintain a current list of its consortium members and communicate any changes to the Secretariat in a timely manner.

<sup>1</sup> The U.S.-China Clean Energy Research Center is a bilateral research initiative to encourage R&D collaboration and accelerate advanced technology development and deployment in both countries. It is organized by the two governments under a Protocol, signed on November 17, 2009. Participating agencies are for the PRC the Ministry of Science and Technology, the National Energy Administration, and the Ministry of Housing Urban and Rural Development and for the U.S. the Department of Energy

<sup>2</sup> Criteria for funding CERC research projects include: (a) scientific and technical merit; (b) relevance to larger thematic objectives; (c) quality of the research team, including its leaders, key research personnel and supporting resources, equipment, and facilities; (d) expected benefits for both countries (not just one country); (e) emphasis on science, technology and innovation, with potential for new intellectual property; (f) path to commercialization of resulting knowledge or technology; and (g) evidence of joint planning and US-China research collaboration.

<sup>3</sup> Protocol and Technology Management Plans may be found at: <http://www.us-china-cerc.org>.

# Appendix E: Advanced Coal Technology Consortium Project Fact Sheets

Advanced Power Generation .....E3

Clean Coal Conversion Technology .....E5

Pre-Combustion CO<sub>2</sub> Capture.....E6

Post-Combustion CO<sub>2</sub> Capture .....E8

Oxy-Combustion CO<sub>2</sub> Capture .....E10

CO<sub>2</sub> Sequestration.....E12

CO<sub>2</sub> Utilization .....E14

Simulation and Assessment .....E15



## Research Topics

The Advanced Coal Technology Consortium (ACTC) focuses on the most critical research needs, categorized by the following eight research thrusts:

1. *Advanced Power Generation*: Develop breakthrough technologies in advanced coal power generation and the application of advanced technology.
2. *Clean Coal Conversion Technology*: Conduct research, development, and demonstration of new coal co-generation systems with CO<sub>2</sub> capture, including new coal-to-chemical co-generation; new CO<sub>2</sub> capture processes; and co-generation systems with combined pyrolysis, gasification, and combustion. Projects in this area will pursue high-efficiency conversion.
3. *Pre-Combustion CO<sub>2</sub> Capture*: Conduct major industrial-scale demonstrations of integrated gasification combined cycle (IGCC) power generation with carbon capture and sequestration.
4. *Post-Combustion CO<sub>2</sub> Capture*: Investigate various technologies for post-combustion capture and conduct demonstrations of CO<sub>2</sub> capture, utilization, and storage in cooperation with large power generation companies.
5. *Oxy-Combustion Research, Development, and Demonstration*: Study the fundamental and pilot-scale combustion and emission characteristics of indigenous Chinese and U.S. coals of different ranks under oxyfuel conditions, create a model for oxy-fired burner design, evaluate and optimize pilot-scale oxy-combustion, and conduct a commercial-scale engineering feasibility study for an oxyfuel-combustion reference plant, with the goal of achieving cost and performance breakthroughs in the laboratory and the field that help overcome the challenges to oxyfiring with both U.S. and Chinese coals.
6. *Sequestration Capacity and Near-Term CCUS Opportunities*: Develop research work focused on CO<sub>2</sub> geological sequestration (CGS) in China's Ordos Basin to better understand and verify key technologies for CO<sub>2</sub> storage in saline formations, to provide the scientific evidence to implement large-scale carbon capture and storage (CCS) in China and to provide support for CCS development in the United States.
7. *CO<sub>2</sub> Algae BioFixation and Use*: Support the industrial demonstration of carbon biofixation using microalgae to absorb CO<sub>2</sub> and turn the biomass produced into a rich source of renewable energy, including biodiesel.
8. *Integrated Industrial Process Modeling and Additional Topics*: Apply modeling techniques to a wide variety of issues associated with pre- and post-combustion CO<sub>2</sub> capture and oxy-combustion in order to assess the economic and operability potential of existing capture technologies in conjunction with removal of criteria pollutants, assess the technical feasibility and potential economic benefit and operability of new, novel carbon capture technologies, and optimize the economics of different carbon capture technologies.

# Advanced Power Generation

U.S. Research Team Lead	China Research Team Lead	
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U.S. Partners	China Partners	
<ul style="list-style-type: none"> <li>• LP Amina</li> <li>• Babcock &amp; Wilcox Power Generation Group, Inc.</li> </ul>	<ul style="list-style-type: none"> <li>• Tsinghua University</li> <li>• Shanghai Jiao Tong University</li> <li>• Harbin Institute of Technologies</li> <li>• Huaneng Clean Energy Research Institute</li> </ul>	<ul style="list-style-type: none"> <li>• China Power Investment Corporation</li> <li>• China Power Engineering Consulting Group Corporation</li> <li>• Shenhua Group</li> </ul>

## Research Objective

The researchers are pursuing activities that will lead to a breakthrough in advanced coal generation and applications of key technologies. There are three categories within this research topic:

### Upgrade pulverizing system for subcritical power plants

- Evaluate potential improvements of coal pulverizers in coal-fired power plants (CFPPs) in China and the United States
- Identify target units from CFPPs with a coal classifier

### Advanced ultra supercritical (A-USC) power generation

- Conduct research on combustion and heat transfer characteristics of large-capacity and high-parameter boilers
- Study the combustion and heat transfer characteristics of super 700°C A-USC boilers
- Establish a prediction model for ash deposition, and provide quantitative data for fine particle removal and ash deposition prevention

### Improve efficiency, availability, and carbon reduction of existing coal-fired power plants

- Obtain detailed data related to increasing efficiency and carbon reduction for different boiler types, loads, and coal types for in-service power plants
- Evaluate the retrofit technologies and obtain the technological roadmap for increasing efficiency and pollutant emission reduction
- Obtain the retrofitting and operation experience of key technologies

## Technical Approach

The technical approach for this project contains three categories:

### Upgrade pulverizing system for subcritical power plants

- Survey the modification of coal pulverizers in coal-fired power plants (CFPPs) in China and the United States
- Evaluate potential improvements, including different configurations of coal mills and the pulverizing system
- Identify target units from CFPPs with a coal classifier

### A-USC boiler development

- Conduct research on a thermodynamic system of 700°C A-USC units combusting Xinjiang coal
- Design a system for 700°C A-USC boilers combusting Xinjiang coal
- Conduct research on heat transfer and hydrodynamics of 700°C A-USC boilers
- Conduct research on fouling and slagging characteristics of 700°C A-USC boilers

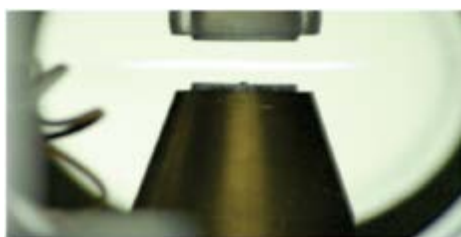
### Improve efficiency, availability, and carbon reduction of existing coal-fired power plants

- Survey operation of existing CFPPs that have adopted efficiency improvement technology both in China and the United States
- Identify one or two specific units (e.g., 300–600 megawatt electrical [MWe]) with similar characteristics in both countries
- Analyze the operational characteristics and cycling behaviors of these plants and conduct a performance diagnosis
- Evaluate the potential for efficiency improvements and emission reduction
- Develop a final toolbox for both China and the United States to use in improving CFPPs

## Recent Progress

In year 2 of CERC, research focused on investigating the combustion of Xinjiang Houxun coal in A-USC boilers. Fundamental experiments were conducted on coal with severe combustion characteristics. The development of improved A-USC boiler technologies was adopted as a national program by China. Also in year 2, LP Amina was able to investigate the current fuel processing system distribution in the United States. Further details on research progress include the following:

- Gathered statistics about type of unit, number, and capacity of CFPPs in China through a survey. The data showed that by the end of 2009, subcritical power plants account for 78% of the coal-fired fleet, while supercritical and ultra supercritical units make up the remaining 22%. It was determined that the target plant for detailed investigation will be a subcritical unit with a capacity range from 300 to 600 MWe
- Finalized the benchmark investigation survey for the target CFPPs, with the following parameters necessary for a complete investigation: design parameters such as steam parameters, furnace and burner design, pulverizing system characteristics, flue-gas temperatures, and soot blowing system details; operational parameters such as heat rate, excess air, and load factor; and information about installing existing energy conservation and emissions reduction technologies such as soot blowing
- Carried out research on pulverized coal combustion in counterflow flames quite successfully. Accomplished the design, processing, assembly, and preliminary test of the first-of-a-kind experimental system
- Studied the ignition in the Hencken burner and investigated different ignition mechanisms, ignition characteristics with a thermogravimetric analyzer/wire mesh reactor, and burnout properties of mixed coal. The research of A-USC power generation was combined with an investigation of the characteristics of Xinjiang coal. Research on combustion and



Figures 1 and 2. Particle behavior during flame penetration is visible.

hydrodynamic coupling characteristics of an A-USC boiler was performed. Theoretical modeling and numerical simulation of the aerial dynamic field, temperature field, and combustion efficiency of an A-USC boiler was completed. Construction of an experimental platform designed to investigate the combustion and hydrodynamic coupling characteristics of a 0.3 megawatt A-USC boiler is in process. The team also conducted an investigation on transformation of minerals in combustion and the characteristics of soot heat resistance. The influence of fouling and slagging on the heat resistance of the heating surface was studied. To identify a methodology for predicting and controlling fouling and slagging, quantum chemistry was introduced

- Investigated the transformation of minerals in combustion and the characteristics of soot heat resistance. The influence of fouling and slagging on the heat resistance of the heating surface was studied. To identify a methodology for predicting and controlling fouling and slagging, quantum chemistry was introduced

- Investigated the influence of the pulverizing system on NO<sub>x</sub> emission; researchers noted that the characteristics of the fuel, the primary air, and the combination of the air and fuel are the dominate influences. Factors such as the oxygen concentration in the burner zone and temperature in the burner zone also affect the emission of NO<sub>x</sub>

#### *Expected Outcomes*

The research team's efforts in A-USC power generation will produce a thermal calculation method of large-capacity and high-parameter boilers, a general large-capacity boiler thermal calculation program module, a calculation method of furnace combustion and heat transfer for super 700°C A-USC boilers, heat transfer coupling characteristics between the furnace and the pipe of USC boilers, and a prediction model of ash fouling and slagging in A-USC boilers.

# Clean Coal Conversion Technology

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>West Virginia University</li> <li>LP Amina</li> <li>National Energy Technology Laboratory</li> <li>Lawrence Livermore National Laboratory</li> <li>University of Wyoming</li> <li>University of Kentucky</li> </ul>	<ul style="list-style-type: none"> <li>Zhejiang University</li> <li>Shenhua Group</li> <li>China University of Mining &amp; Technology</li> <li>ENN (XinAo Group)</li> <li>China Academy of Sciences</li> </ul>

## Research Objective

Collaborative research teams from the United States and China are performing research and development (R&D) of new coal co-generation systems with CO<sub>2</sub> capture, including new coal-to-chemical co-generation; new CO<sub>2</sub> capture processes; and co-generation systems with combined pyrolysis, gasification, and combustion. Specifically, the team will accomplish the following:

- Develop and deploy a new poly-generation technology to reduce waste heat, water utilization, and greenhouse gas emissions while improving thermal efficiency in utilization of coal to produce power and chemical by-products
- Design and build a demonstration coal-to-chemicals poly-generation plant in China under the leadership of LP Amina to demonstrate the new poly-generation technology
- Conduct R&D of new coal co-generation systems with CO<sub>2</sub> capture, including new approaches for coal-to-chemical co-generation

## Technical Approach

Researchers from both countries are working together to develop new technology to convert conventional power plants into poly-generation plants that make full use of waste heat and oxy-fuel combustion to produce chemicals and further polymers from coal. The approach leverages investments in technology development and industrial implementation aimed at reducing emissions, improving efficiency, and increasing economic benefits associated with coal power production. The technical approach includes the following:

- Build a laboratory-scale research facility
- Develop a new carbothermic reduction process to produce standard industry chemicals from limestone and coal
- Produce synthetic chemicals and fuels

This research will result in the development of a demonstration project at a power plant in Shanxi, China, by LP Amina. In addition to standard engineering analysis, this work will require a substantial amount of basic research, especially in system analysis, reactor dynamics, chemical kinetics, emissions, and process stability and reliability.

## Recent Progress

Researchers from the Chinese and U.S. teams have carried out the related R&D efforts smoothly and achieved meaningful progress on co-generation system combined pyrolysis, gasification, and combustion; chemical looping gasification with CO<sub>2</sub> capture; direct synthetic natural gas (SNG) production from coal; gasification properties of the coal direct liquefaction residue; measurement, modeling, and environmental technologies for unconventional coal gasification; and the coal/biomass co-conversion process. Researchers have accomplished the following major achievements:

- Validated coal co-generation technology combined pyrolysis, gasification, and combustion on a 1 megawatt thermal pilot plant; this technology may be demonstrated in industry
- Completed commissioning tests of the constructed ~15 kilograms/hour chemical looping gasification facility and validated the coal chemical looping gasification technology approach
- Obtained coal gas with high-concentration CH<sub>4</sub> from the constructed bench-scale high-pressure constant volume reactor, which validated the possibility of direct SNG production from coal
- Confirmed the feasibility of liquefaction residue for coal gasification and developed suitable additives for coal liquefaction residue and coal mixture slurries

- Utilized a model underground coal gasification test reactor to evaluate the temperature and concentration fields and to draw a model of the cavity
- Developed the key processes and efficient catalyst for co-transformation of biomass and coal based on the constructed experimental platform

## Expected Outcomes

The implementation of poly-generation will reduce capital costs, greenhouse gas emissions, and plant maintenance costs of power generation sites. When paired with cleaner coal utilization with increased efficiency and minimal waste, poly-generation will be a cost-effective, commercially viable option for reducing CO<sub>2</sub> emissions in the power generation sector. This approach will also enable minimization of waste heat and/or materials. The LP Amina-Gemeng International Energy plant could reduce greenhouse gases compared to conventional technology by more than 25%.



Figure 1. Coal-fired furnace.



# Pre-Combustion CO<sub>2</sub> Capture

U.S. Research Team Lead	China Research Team Lead
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## Research Objective

The development and implementation of the integrated coal gasification combined cycle (IGCC) into power generation is still in the first-of-the-kind stages. In this theme, industrial, research, and academic leaders from both the United States and China will work with industrial-scale demonstration projects and best-in-class technologies to provide the world with robust, transparent cost and performance estimates for IGCC power plants with carbon capture and storage (CCS).

This project has one primary goal: development of techniques to aid in the design and optimization of commercial-scale IGCC systems. Specifically, the team will accomplish the following:

- Assess the economic feasibility and operability of gasification technologies in conjunction with the removal of criteria pollutants
- Assess the technical/economic feasibility and operability of novel carbon capture technologies
- Optimize the economics of different carbon capture technologies
- Establish guidelines/protocols/criteria for system optimization and evaluation, as well as techno-economic analysis and comparison at commercial-scale application

## Technical Approach

The project emphasizes system integration, optimization, and key component development. The technical approaches for the project's two tasks are the following:

Development of techniques for integration and optimization of an IGCC system

- Study the integration, optimization, and modular design of an IGCC system based on the existing research and demonstration experience of the first IGCC plant in China, as well as the experience of both existing and under-construction IGCC in the United States

Understand the key components in a pre-combustion CO<sub>2</sub> capture process

- Design and construct the slipstream-scale pre-combustion CO<sub>2</sub> capture and utilization system by extracting a slip-stream syngas from an existing IGCC plant

To accomplish this work, researchers (led by the China Huaneng Group and assisted by Duke Energy in the United States) will develop techniques for the optimization and design of a commercial-scale IGCC system based on the existing research and demonstration experience of GreenGen, the first IGCC plant in China, and the experience of IGCC at Duke Energy's Edwardsport Station.

The major obstacles the two companies have been trying to work through include various intellectual property issues and other legal issues with the partners providing the technology.

Researchers (led by Huaneng) will also develop advanced key components including pre-combustion CO<sub>2</sub> capture featuring heat-integrated, robust, ultrathin barriers with reasonable contamination resistance to flue gas; advanced water-gas shift reactors; advanced separation reagents; and advanced compression technology.

The ACTC team's specific activities that further pre-combustion CO<sub>2</sub> capture will include the following:

- Developing and fabricating heat-integrated, robust, ultrathin barriers with reasonable contamination resistance to flue gas for both pre- and post-combustion CO<sub>2</sub> removal
- Formulating new CO<sub>2</sub> absorbents with chemical additives for pre- and post-combustion CO<sub>2</sub> capture with high capacity, fast kinetics, and high stability
- Initializing models for existing pre-combustion capture technologies, chiefly physical sorbents, both as individual models and within the two reference plants (including water-gas shift and gas cleanup)

## Recent Progress

Duke Energy's Edwardsport plant and Huaneng's GreenGen IGCC reached an agreement on the reporting format and identified that information regarding the following example areas will be exchanged:

- Air separation unit
- Gasification
- Power block
- General utilities and common systems
- Environmental performance
- High-level costs
- Start-up report

Both companies would prefer to hold a workshop at each owner's IGCC site, as well as develop a long-term IGCC technology-sharing relationship. There are significant intellectual property issues that will need resolution before a long-term agreement can be developed.

The ACTC team's specific progress for pre-combustion CO<sub>2</sub> capture research includes the following:

- Completed the comparison, selection, and unit modeling of a 30 megawatt thermal (MWth) pre-combustion CO<sub>2</sub> capture system
- Completed the process flow diagram, which includes the equipment layout, process equipment tables, major static equipment diagrams, and system control program. Completed the key equipment design of a 30 MWth CO<sub>2</sub> capture system based on IGCC
- Completed the capture reagent and process development evaluation. Confirmed the best adsorption temperature and the fittest CO<sub>2</sub> concentration of CaCO<sub>3</sub> and CaC<sub>2</sub>O<sub>4</sub> as precursors
- The high-temperature, solid-state method is used to modify the adsorbent by doping magnesium, aluminum, cerium, zirconium, and lanthanum. The team found that the adsorption capacity was dependent on different conditions

### *Expected Outcomes*

Key outcomes will include critical data, lessons, and knowledge shared through operational experience with demonstration projects as systems are optimized and the cost of pre-combustion CO<sub>2</sub> capture is lowered. Such knowledge sharing contributes to accelerating the development of IGCC with CCS, a critical pathway toward low-carbon power generation with coal.



Figure 1. Duke Energy Edwardsport IGCC.



Figure 2. China Huaneng GreenGen IGCC.

# Post-Combustion CO<sub>2</sub> Capture

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Kentucky</li> <li>University of Wyoming</li> <li>Los Alamos National Laboratory</li> <li>Lawrence Livermore National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>China Huaneng Group Clean Energy Research Institute</li> <li>Tsinghua University</li> <li>China Power Engineering Consulting Group Corporation</li> <li>China Power Investment Corporation</li> </ul>

## Research Objective

The goal of this task is to integrate new capture and solvent technologies into the development of efficient CO<sub>2</sub> capture. Parts or combinations of these technologies will be used to lower the energy costs related to a post-combustion capture process.

The Advanced Coal Technology Consortium (ACTC) team is directly addressing the need for steep emissions reductions from the existing coal fleet by analyzing, testing, and demonstrating technologies for post-combustion capture integrated with sequestration at real power plants. Through streamlined bilateral joint cooperation, U.S. and Chinese researchers are looking to accomplish the following:

- Research efficiency developments for affordable post-combustion CO<sub>2</sub> capture technologies
- Coordinate efforts between U.S. and Chinese partners
- Develop models for post-combustion CO<sub>2</sub> capture, utilization, and storage (CCUS) technology at a commercial scale

## Technical Approach

To enable commercial-scale CCUS, the ACTC team is addressing the gap between theoretical efficiency for post-combustion capture and present-day commercially available technologies. The team's technical approach includes the following:

- Conduct a pre-engineering study of the 1 million tons/year post-combustion CO<sub>2</sub> capture systems, combined with a preliminary techno-economic analysis and budgetary cost estimate ( $\pm 30\%$ ). Upon completion, a sensitivity study of power generation with a post-combustion carbon capture system will be performed

- Develop innovative solvent compositions to reduce the overall cost of carbon capture and storage (CCS) in three steps: (1) establish a performance matrix for solvent formulation and evaluation, (2) formulate the solvent, and (3) conduct evaluations at various levels of scale to determine the solvent's performance capabilities compared to the matrix
- Use rational design for future catalyst generation, building on the success of previous Center for Applied Energy Research (CAER) catalysts to enhance the CO<sub>2</sub> mass transfer rate in CO<sub>2</sub> amine solutions used for post-combustion capture, to demonstrate catalyst stability and robustness under conditions conducive to post-combustion carbon capture, and to demonstrate catalyst performance in a capture process using coal-derived flue gas
- Develop high-throughput CO<sub>2</sub> capture membranes, leading to improved capture efficiency and reduced capture costs via the design and synthesis of highly CO<sub>2</sub>-permselective polyethylene-glycol-based hybrid membrane materials; development of novel methods based on ultrasonically assisted deposition techniques to fabricate ultrathin composite membranes with unprecedented high CO<sub>2</sub> permeances on commercially attractive support platforms; and demonstration of these developed materials and methods via membrane separation evaluations under industrially relevant coal-derived flue gas conditions
- Investigate the use of carbon xerogel and surface-modified carbon xerogel for the enrichment of carbon-loaded monoethanolamine (MEA) species



Figure 1. Piping network in an existing coal power plant.



### Recent Progress

The research team completed the conceptual simulation for a 1 million tons/year post-combustion CCS project in Gibson-3.

Researchers started a demonstration project at Duke Energy's Gibson station, where the current cost of CO<sub>2</sub> capture can be effectively evaluated. Catalyst and solvent development will be used to not only prolong the life of the capture solvent, but also to increase mass transfer into the liquid phase, thereby decreasing the size of the absorber necessary in the capture process. The carbon loadings of the solvent will also be increased through the use of blended solvents.

Researchers also developed a two-phase solvent for CO<sub>2</sub> capture. They screened the two-phase solvent, analyzed the two-phase mechanism, and analyzed the product. The work has involved the demonstration of the process using a laboratory-scale absorption/desorption column to yield cyclic capacity for various solvent blend compositions. The speciation in the two solvent phases was identified and demonstrated the loading of CO<sub>2</sub> in each phase.

The U.S. side has been focused on the development of catalysts capable of withstanding the harsh conditions associated with carbon capture, and it favors bicarbonate dissociation to regenerate the active catalyst. The work has involved demonstration of a new class of catalyst with record-breaking activity on the bench scale using the pH-drop, CO<sub>2</sub> breakthrough, and a wetted wall column. Catalyst stability has also been established at the laboratory scale to high-temperature operation and multiple absorption/desorption cycles.

The U.S. side's efforts are additionally focused on development and demonstration of hybrid CO<sub>2</sub> selective membrane materials that exceed the CO<sub>2</sub> permeance performance of previously developed membranes. Methods to deposit ultrathin selective layers of these hybrid materials on commercially attractive supports have been developed and are under continued optimization. This deposition work is closely coupled with the site's materials design efforts and is aimed at realizing production of viable

fabrication methodologies for the developed membrane materials. These efforts incorporate assessment of material and membrane properties relevant to the long-term stability, durability, and separation performance of the developed technology in industrially relevant environments.

A series of candidate catalysts were computationally modeled, guided by previous catalyst results. It was previously concluded, based on computational transition state modeling, that compounds with long Zn–O yet low (<8.5) pKa are needed. Longer Zn–(OH–) bonds lead to the following:

- Lower Lewis acidity of the metal-ligand complex
- More of a “free” hydroxide (and more nucleophilic)
- Higher pKa for the H<sub>2</sub>O deprotonation step

The team also developed an ultra-sonic atomization-based coating technique to fabricate an ultrathin selective layer on commercially attractive porous supports.

Researchers completed project objectives for the year, including evaluating a catalyst in conditions conducive to carbon capture; identifying a discrepancy between pH-drop and stopped flow; performing density field theory (DFT) calculations; and synthesizing and evaluating a new catalyst. Further refining the conclusion from last year based on experimental results, the lack of activity of the Zn(cyclen) catalyst is believed to be caused by salt exchange bringing anions into the secondary coordination sphere. This inhibits regeneration of the active species. The new complexes utilizing the ligands LP and LS1 alleviate this problem and allow for an improvement in CO<sub>2</sub> hydration activity.

Work on capacitive deionization (CDI) for MEA solvent enrichment has focused on the development of highly conductive, porous carbon xerogel materials as well as modifying the surface chemistry of these carbons to increase the enrichment efficiency. CDI has been shown to successfully concentrate MEA molecules, with further developments needed to lower energy costs and increase efficiencies.

### Expected Outcomes

All of the research in this project will be used to show that the energy cost of CO<sub>2</sub> separation from current power plants and the capital cost of the process equipment can be dramatically decreased.

The project will produce optimized design options of competing technology pathways (e.g., amines and advanced solvent) for post-combustion CCUS cost, retrofitability, engineering, and environmental performance. The results from this work will lay the groundwork for decision makers in both China and the United States to understand the potential role of post-combustion retrofits in achieving steep reductions, as well as provide new operational insights on the integration of capture and storage while developing new low-cost, post-combustion capture options.

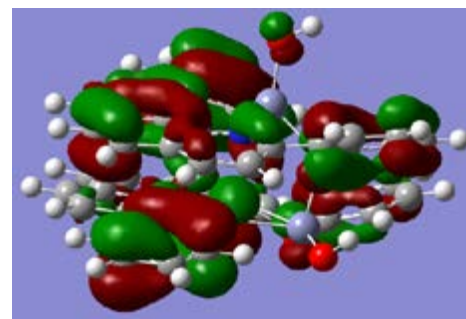


Figure 2. Density field theory (DFT) calculations of the electronic structure (HOMO) for a representative CAER-developed catalyst.

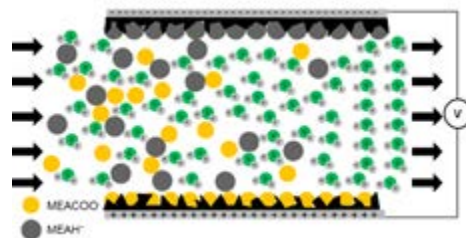


Figure 3. Schematic representation of capacitive-deionization-based amine solvent enrichment.



# Oxy-Combustion CO<sub>2</sub> Capture

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## Research Objective

Researchers from the U.S.-China Advanced Coal Technology Consortium (led by the Huazhong University of Science and Technology [HUST] in China and by Babcock & Wilcox [B&W] in United States) will collect fundamental and pilot-scale data associated with various oxy-combustion conditions and conduct feasibility and economic analysis on the commercial-scale deployment of the technology for CO<sub>2</sub> capture. The objectives for Theme 5 activities are defined as follows:

- Determine combustion and emission characteristics of indigenous Chinese and U.S. coals of different ranks under oxy-combustion conditions
- Evaluate and optimize pilot-scale oxy-combustion technology
- Develop a computational fluid dynamics (CFD) and process model for oxy-combustion
- Enable knowledge sharing on the feasibility study of the large-scale demonstration

## Technical Approach

With experience from previous U.S. work, along with the development of new research pilots in China, an opportunity exists to accelerate the path to commercialization and broaden the application across regions and fuel types. The primary approach focuses on expanding the experience of oxy-combustion into broader applications in the United States and China. The technical approach comprises four main activities:

Fuel characterization and hazardous air pollution emission study under oxy-fuel conditions

- Conduct analysis of representative samples of different ranks of Chinese and U.S. coals
- Conduct experiments on characteristics of coal pyrolysis, ignition, combustion, burn off, dust stratification, slagging, and deposition in bench-scale facilities. Also, conduct tests on NO<sub>x</sub> formation and destruction, PM<sub>2.5</sub> emission, and control

- Develop and implement reaction chemistry sub-models on combustion and NO<sub>x</sub> formation under oxy-combustion conditions to provide a tool for burner design and oxygen injection optimization (HUST's Furnace Model [FURN]) and B&W's Combustion Model [COMO])

Pilot-scale oxy-fuel combustion evaluation and optimization

- Carry out pilot-scale tests in research facilities at B&W and HUST using selected Chinese and U.S. coals
- Configure the research facilities at B&W and HUST for the optimum oxy-combustion flue gas recycling process (e.g., warm-recycle, cool-recycle, or cold-recycle) using a new burner design
- Collect performance data on combustion, heat transfer, furnace exit gas temperature, and emissions over a wide range of practical operating conditions
- Select the most promising design, based on modeling predictions and performance criteria for further demonstration

Steady-state and dynamic process modeling simulations

- Compare Aspen Plus static predictions with pilot-scale data
- Use Aspen Plus Dynamics to simulate transient oxy-combustion processes
- Validate and tune the dynamic process model toward developing a control strategy for start-up, shutdown, modulations, and unit trips (e.g., boiler, air separation unit, and compression and purification unit)

Feasibility study for large-scale deployment

- Facilitate information exchange on policy, investment, and technical issues to conduct a feasibility study of a reference wall-fired pulverized-coal-burning unit for oxy-combustion
- Perform unit and process concept reviews of the air separation unit, boiler island, compression and purification unit, and the balance of plant

## Recent Progress

HUST and B&W signed a research collaboration agreement in June 2012. The two sides held two technical discussion sessions in 2012. Monthly teleconferences were started in September 2012.

In 2012, four U.S. and four Chinese coals were characterized. Researchers identified the importance of char gasification with CO<sub>2</sub> and H<sub>2</sub>O for low-rank coals under oxy-combustion conditions. Based on the experimental results, researchers optimized reaction rate parameters in a char burnout sub-model in the CFD code.

CFD models for both HUST's full chain system (FCS) and B&W's small-boiler simulator (SBS) pilot-scale test facilities were developed for B&W's COMO and HUST's FURN codes. Researchers set up and carried out three simulation cases for the SBS—two air-firing and one oxy-firing. They also identified three simulation cases—one air-firing and two oxy-firing—for the FCS facility. Simulation efforts are currently underway.

Researchers also carried out preliminary development of Aspen steady-state and dynamic models for SBS and FCS. B&W issued the work plan and programmer's guide for the SBS steady-state process model. HUST conducted a dynamic simulation study of FCS oxy-firing transitions.

## Expected Outcomes

This project will lead to cost and performance improvements that are rooted in fundamental science from testing in the laboratory and the field. The use of computer simulation and modeling will allow for greater progress on future demonstrations by reducing risk and optimizing both design and critical areas that require large-scale validation. Ultimately, the economic and environmental potential of oxy-firing combustion will be attributable to a wider range of solid fuels and at a commercially viable scale. The use of the computer models, once validated at large-scale commercial projects, will reduce the risk of deployment and increase

the speed of deployment for a wide variety of world coals that normally present additional challenges. These small-scale pilots and the computer models will then become a valuable tool for faster deployment of cutting-edge technology in a long-lived, capital-intensive market space.

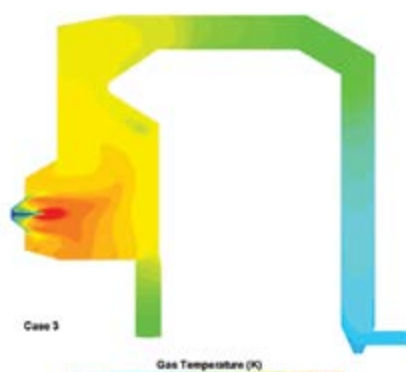


Figure 1. B&W small-boiler simulator oxy-coal temperature map.

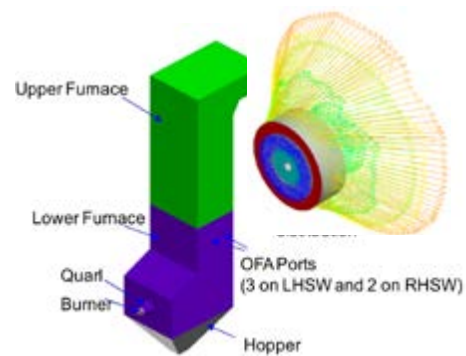


Figure 2. HUST full chain system.



Figure 3. Chinese and U.S. research pilots.

# CO<sub>2</sub> Sequestration

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• University of Wyoming</li> <li>• Los Alamos National Laboratory</li> <li>• Lawrence Livermore National Laboratory</li> <li>• Indiana Geological Survey</li> <li>• West Virginia University</li> </ul>	<ul style="list-style-type: none"> <li>• Shaanxi Provincial Institute of Energy Resources</li> <li>• Yanchang Petroleum Group</li> <li>• Institute of Rock and Soil Mechanics, Chinese Academy of Sciences</li> <li>• Shenhua Group</li> <li>• Qinghua University</li> <li>• China University of Mining and Technology, Beijing</li> <li>• China University of Mining and Technology, Xuzhou</li> </ul>

## Research Objective

This theme's research is focused on estimating the CO<sub>2</sub> storage capacity of the Ordos Basin, China, and identifying near-term opportunities for geological CO<sub>2</sub> storage (carbon capture and storage [CCS] and carbon capture, utilization, and storage [CCUS]). This effort includes the following:

- Characterize targeted geological storage reservoirs in three dimensions, on both regional and site-specific scales, based on all available public geological, geophysical, geochemical, petrophysical, petrographic, and petroleum engineering data. This research is especially concerned with characterizing reservoir and seal heterogeneity, as well as the effects of heterogeneity on CO<sub>2</sub> injectivity and storage capacity assessments
- Develop the scientific, technological, and engineering framework required for CO<sub>2</sub> utilization in the Ordos Basin via enhanced oil recovery (EOR). The utilization strategy will include safe, permanent storage of large quantities of anthropogenic CO<sub>2</sub>
- Develop simulation technology for CO<sub>2</sub> storage in saline formations
- Research and apply monitoring technology of CO<sub>2</sub> storage in saline formations
- Assess safety and risk of CO<sub>2</sub> storage in saline formations
- Understand system feedbacks, including the impacts of source locations on optimization of storage systems
- Conduct geological characterization

Through combined research on these issues and successful execution of demonstration projects, this effort will improve understanding, provide verification of key technologies for CO<sub>2</sub> storage in saline formations, and provide the scientific evidence to implement large-scale CCS and CCUS in China and the United States.

The project has two primary objectives:

- Build the scientific, technological, and engineering framework necessary for CO<sub>2</sub> utilization through EOR and the safe, permanent storage of commercial quantities of anthropogenic CO<sub>2</sub> in the Majiagou Limestone of the Ordos Basin, Shaanxi Province, China
- Assess the safety and risk of CO<sub>2</sub> storage in saline formations

## Technical Approach

In the near-term (2013), the team plans to accelerate data collection and move forward with work in the Ordos Basin (China), the Illinois Basin, and the Green River Basin (Rock Springs Uplift) in Wyoming. Both the United States and China are struggling to determine what data can be released publicly to facilitate collaboration that will allow use of the best algorithms from both China and the United States. Thus, an objective for 2013 is to generate regional-scale data from publicly available sources that can be shared between both countries. The team continues to monitor the progress of developments in the coal-to-liquid industry in the Ordos Basin.

Collaboration at the site scale will require application-dependent cooperation that may or may not involve direct sharing of sensitive data. Sharing executable algorithms will allow teams on either side to create results using the range of tools available to the U.S.-China Clean Energy Research Center (CERC). The team will continue

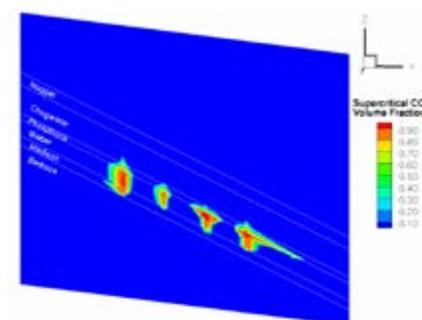


Figure 1. Illustrative simulation model output for supercritical CO<sub>2</sub> volume fraction.

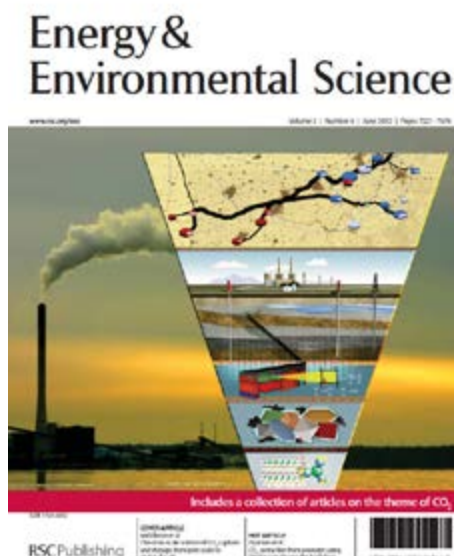


Figure 2. Journal cover tied to CERC work on optimizing pipeline networks from CO<sub>2</sub> sources to CO<sub>2</sub> storage reservoirs.

to pursue opportunities to exchange personnel to increase productivity and joint understanding of algorithm implementation.

Both U.S. and Chinese teams will continue to develop models for specific sites in their own countries that will support the overall goals of the project without constraints. Specifically, using the University of Wyoming projects as analogs, the team proposes to work closely with research scientists from the Shaanxi Provincial Institute of Energy Resources and Chemical Engineering and Northwest University to assess the anthropogenic CO<sub>2</sub> resources and geological CO<sub>2</sub> storage capacity of the Ordos Basin.

The Yangchang Oil Company plans to initiate a CO<sub>2</sub> storage and CO<sub>2</sub>-EOR project this summer. Company representatives plan to visit Wyoming in early summer to seek assistance with project design (e.g., reservoir heterogeneity characterization, structural and property modeling, injection and production simulation, economic evaluation). The joint project team has arranged a joint field trip in the Ordos Basin this summer to study the targeted storage reservoirs and potential sealing strata, and to observe cores in the Yanchang and North China Oil Company core repository. To assist the Yangchang Oil Company with its CO<sub>2</sub>-EOR and storage demonstration projects, the team is planning a trip to work on the reservoir data at the Yangchang facility in order to continue to build structural and property models. Using these models, the team will perform numerical simulations for the targeted reservoir and storage site at facilities in Wyoming.

Detailed three-dimensional geological, structural, and property models will be constructed for the selected mature oil reservoir (i.e., targeted CO<sub>2</sub> flooding reservoir). Reservoir heterogeneity will be built into these models using outcrop and core observations, well log analyses, seismic interpretations, and Wyoming analogs.

### *Recent Progress*

In the last year, the partners from Northwest University, Shaanxi Provincial Institute of Energy Resources and Chemical Engineering, the Yangchang Petroleum Company, the North China Oil Company, the Institute of Rock and Soil Mechanics, China University of Mining and Technology, the University of Wyoming, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, the Indiana Geological Survey, and West Virginia University have accomplished the following tasks:

- Assembled a large set of information regarding the geologic, petrophysical structural/stratigraphic frameworks of the Ordos Basin, Rock Springs Uplift, and Illinois Basin
- Inventoried the distribution of fossil energy and anthropogenic CO<sub>2</sub> resources in the Ordos Basin
- Delineated CO<sub>2</sub> sources and sinks in the Illinois Basin, the Ordos Basin, and sources for Wyoming
- Explored the potential of developing CCUS analogs between the Ordos Basin and the Powder River/Green River Basin and Illinois Basin using the latest screening criteria
- Published results from a numerical study of CO<sub>2</sub> injectivity, storage capacity, and leakage for the Rock Springs Uplift in Wyoming in the International Journal of Greenhouse Gas Control (Impact factor 5, Figure 2)
- Published results from an analysis of the impacts of CO<sub>2</sub> source variability on storage costs in Applied Energy (Impact factor 5)
- Published a methodology for regional-scale system analysis using data from the southeast United States in Energy & Environmental Science (Impact factor 9.5, Figure 3); methodology adapted partially from National Risk Assessment Partnership (NRAP) and applied to the Gibson site to emulate multiphase flow and reactive transport

- Developed site prioritization methods and ranked saline storage reservoirs
- Leveraged collaboration between the Yangchang Oil Company and the Theme 6 team to initiate design, construction, and injection at a pilot CO<sub>2</sub>-EOR project in the Ordos Basin

### *Expected Outcomes*

The significant opportunity for storage and utilization of CO<sub>2</sub> in the Ordos Basin in China complements opportunities that are being explored in basins in the United States, such as in Wyoming and Illinois. The research team is looking at the Ordos Basin in parallel to this research.

The lessons learned will be invaluable to CCS projects, particularly in Rocky Mountain basins; the Majiagou Limestone and Ordos Basin are very similar to the Paleozoic Madison Limestone and the Powder River Basin of Wyoming and Montana.

This work ultimately improves global understanding of how to safely and effectively store CO<sub>2</sub> in saline formations or to use the CO<sub>2</sub> for EOR.

The most important outcomes at the end of Year 5 are expected as follows:

- Jointly developed structural, property, and numerical models (including the heterogeneity of the reservoir/seal system) for the highest-priority geological CO<sub>2</sub> storage reservoirs and sites in the Ordos, Green River, and Illinois basins
- A detailed evaluation of all anthropogenic CO<sub>2</sub> sources and sinks in the Ordos, Green River, and Illinois basins
- Initial optimization strategies for pipeline networks in the same basins
- A demonstration project, developed in cooperation with Theme 6 partners, to evaluate the potential of integrated geological CO<sub>2</sub> storage with EOR using CO<sub>2</sub> flooding



# CO<sub>2</sub> Utilization

U.S. Research Team Lead	China Research Team Lead
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## Research Objective

The objectives of this project are to develop and demonstrate an economically feasible technology for CO<sub>2</sub> utilization with microalgae and to transform algal biomass into a sustainable source of energy.

This project aims to accomplish the following sequential goals:

- Identify and culture optimal summer and winter algae strains to be used in the CO<sub>2</sub> mitigation system
- Optimize the culturing process and technology; this should include a demonstration of algae cultivation at pilot-plant scale under summer and winter conditions, incorporating optimized nutrient and water recycling
- Identify and evaluate the possible co-products from the process, including fuels and animal feed
- Use the data gained to construct a techno-economic model to estimate the overall cost of CO<sub>2</sub> fixation and utilization at various scales of operation

## Technical Approach

The work plan is divided into four main tasks: screening algae strains; optimizing the growth system; developing efficient, cost-effective post-processing technologies; and conducting techno-economic analysis. The ongoing tasks include the following:

- Optimize the gene transformation method
- Optimize water recycling
- Optimize nutrient recycling; for example, from anaerobic digestion of harvested algae
- Demonstrate winter operation
- Develop an efficient and effective extraction technology suited for the selected algal species
- Develop a cost-competitive harvesting and dewatering technology with minimal process energy intensity
- Evaluate anaerobic digestion of algae for biogas production

- Conduct economic analysis of the possible power plant savings and costs associated with CO<sub>2</sub> utilization by microalgae

## Recent Progress

The oil-rich microalgae ENN11 was used as an initial strain; after three times ethylmethanesulfonate (EMS) mutagenesis, 2,460 mutants were obtained with temperature and Treatment A tolerance. Researchers selected six high-performance strains, with high growth rate and tolerance to extreme conditions. Researchers also constructed the related plasmids. The construct can overexpress the gene diglyceride acyltransferase (DGAT) from different organisms, which is the key enzyme for triacylglyceride (TAG) biosynthesis, also the step-limit enzyme for the pathway.

The research team designed open-pond and closed photobioreactors to obtain optimal growth physiology and metabolite production at reduced capital and labor costs. The team also optimized culture process for both closed photobioreactors and open-pond photobioreactors, prevented algae culture from experiencing contamination and adhesion, and maintained the algae culture in suitable activity and concentration. After optimization, the outdoor productivity of microalgae biomass was respectively 26 grams/square meter/day (g/m<sup>2</sup>/d) and 22 g/m<sup>2</sup>/d using glass-panel photobioreactors and plastic membrane bioreactors. In pilot experiments, the microalgae productivity of the raceway pond was about 12 g/m<sup>2</sup>/d.

During the second half of 2012, the demonstration facility at East Bend power plant (Kentucky) was constructed, tested, and subsequently seeded (in December) with *Scenedesmus* algae in order to commence a winter growth study. Despite low temperatures, limited sunlight, and problems with the flue gas supply, the algal culture nevertheless showed limited growth. Studies are planned to continue throughout 2013.

Researchers investigated multiple extraction approaches for wet algae extraction technology suited for the selected algal species and growth status. In preliminary experiments, researchers selected four possible wet algae oil extraction methods. Based on a comprehensive evaluation



Figure 1. Demonstration facility installed at Duke Energy's East Bend power plant (Rabbit Hash, Kentucky).

of the selected methods, the M1 and M2 methods were selected for further development for industrial application. Using methods M1 and M2, researchers extracted more than 85% of the total oil and obtained good separation of the oil and water phases. The peroxide value was low, although the acid value was relatively high.

The team completed research concerning the surface features of the selected microalgae ENN11, such as cell morphology, size, surface Zeta charge, and cell sedimentation properties. By adjusting the pH to 10.3 or Fe<sup>3+</sup> to 17 milligrams/liter, the microalgae cell surface Zeta potential went to zero, and microalgae flocculation was achieved.

## Expected Outcomes

Process data (CO<sub>2</sub> capture efficiency, areal biomass productivity, energy consumption, nutrient consumption, etc.) will be collected at the East Bend demonstration installation throughout the second and third quarters of 2013. The accumulated data will be incorporated in a techno-economic model that will enable the costs associated with CO<sub>2</sub> capture and utilization to be calculated at different operating scales; in this manner, potential economies of scale will be identified. Data sharing between the University of Kentucky and Duke/ENN will enable a range of process configurations to be assessed (e.g., open-pond cultivation systems versus closed-loop photobioreactors).

# Simulation and Assessment

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U.S. Partners	China Partners
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## Research Objective

The objectives for this project are to apply modeling techniques to a wide variety of issues associated with pre- and post-combustion CO<sub>2</sub> capture and oxy-combustion in order to accomplish the following:

- Assess the economic and operability potential of existing capture technologies in conjunction with the removal of criteria pollutants
- Assess the technical feasibility and potential economic benefit and operability of novel carbon capture technologies
- Optimize the economics of different carbon capture technologies

## Technical Approach

On the U.S. side, three main subtasks have been identified:

### Power plant cycling and load-following operation

This is a new task, and the U.S. Department of Energy's (DOE's) National Energy Technology Laboratory is focused on determining the effect that power plant cycling and load following have on the life and maintenance of the plant and how improved strategies can be implemented to prolong the life and reduce the maintenance needed for these facilities.

### Systems modeling of post-combustion capture technology

This task involves plant-wide steady-state and dynamic modeling of multiple trains of CO<sub>2</sub> capture equipment. It is focused on the steady-state and dynamic simulation of post-combustion carbon capture processes. The major focus of this part of the work will be to formulate optimal control strategies for multi-train, amine-based processes faced with process disturbances and changes in base loading.

### Initialization of dynamic model with immersive visualization

This task involves implementation of a three-dimensional (3D) immersive training system for an integrated coal gasification combined cycle (IGCC) operator training system. It is focused on upgrading the facilities at the West Virginia University (WVU) Advanced Virtual Energy Simulation Training and Research (AVESTAR) Center to provide full 3D immersive training capabilities for the IGCC operator training simulator. The purpose of this work is to develop training materials to enable industry and universities to have a better understanding of coal-based carbon capture power generating systems.

## Recent Progress

Researchers simulated a steady-state base case based on Cost and Performance Baseline for Fossil Energy Power Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity (November 2010, DOE). The simulation was based on the monoethanol amine (MEA) solvent case for CO<sub>2</sub> capture from a supercritical pulverized coal power plant. A converged steady-state solution (Aspen Plus) was obtained and then a parametric optimization was applied; the net result of this optimization was a reduction in the energy penalty from 12.7 to 10.2 percentage points and a resulting value of 3.07 gigajoules/ton for the heat duty per ton of CO<sub>2</sub> recovered. This optimized case was used as the starting point to generate a pressure-driven dynamic model using Aspen Plus Dynamics. Researchers converged the dynamic model, and the steady-state results compared well with the results from the dynamic simulation. A presentation covering the results of this work was made at the annual American Institute of Chemical Engineers meeting in Pittsburgh.

Researchers developed a dynamic model for a CO<sub>2</sub> capture process with MEA solution, as well as a tower model for the CO<sub>2</sub> absorption and regeneration processes based on gas-liquid phase equilibrium and stage efficiency. An absorber or a stripper is divided into several stages along its height, and in each stage gas and liquid phase equilibrium equations are constructed. A uniform property

assumption is made for each stage; in other words, temperature and pressure is the same everywhere within a stage. Stages are connected via flows of gas and liquid, and via pressure drops. The dynamic model is built on the Dynsim simulation platform, which is a powerful tool for dynamic process simulation. Simulation results of the dynamic model were compared with real-life data and static simulation results (via Aspen) of a pilot power plant with carbon capture at the University of Texas, Austin. Comparison results showed that the dynamic simulation results fit well with the operational data and static simulation results. Dynamic behaviors of a CO<sub>2</sub> absorption process were then studied by adjusting flow rates of flue gas separately, flow rates of lean solution separately, and both simultaneously. Results showed that the process is more sensitive to changes in flow rates of lean solution, and that large changes in flow rates of lean solution (greater than 20%) could lead to unstable operation. It was suggested that a relatively stable ratio between these two flow rates should be kept if the flow rate of one or two of these flows have to be changed.

The software licenses and all necessary hardware for post-combustion capture system modeling were specified and purchased for the implementation of the 3D immersive training system at WVU. The hardware was successfully connected, and the system was commissioned and is operational.

The researchers conducted performance comparison of three retrofitting plans for CO<sub>2</sub> capture: throttle valve, sliding pressure operation, and adding back-pressure turbines. Three retrofitting plans have been proposed to provide heat for CO<sub>2</sub> capture by extracting steam from a steam turbine. Plan A adds a throttle valve between an intermediate-pressure turbine and a low-pressure turbine. Plan B uses an intermediate-pressure turbine to operate at sliding pressure mode by changing its blades at the last stage. Plan C replaces low-pressure turbines with back-pressure turbines. Power generation, power supply, power consumed by compression, and power consumed by

other auxiliary machinery in the three plans are provided. Results show that Plan C has the highest energy efficiency.

The team also conducted a performance comparison of IGCC plants with ion transport membrane (ITM) air separation and cryogenic air separation. Comparison results show that an IGCC plant with ITM air separation is superior on all fronts to an IGCC plant with cryogenic air separation. Increasing the integration degree and high-temperature nitrogen re-injection can lead to even higher energy efficiency.

Researchers developed the modular models of key functional blocks of IGCC plants. Modular models for coal gasification, air separation, sulphur removal, and combine cycle were

developed with consideration of integration between these units. A case study was developed using a 9F gas turbine.

#### *Expected Outcomes*

Application of advanced modeling and simulation tools (e.g., dynamic simulation and  $H_{\infty}$  control) will enable improvements in technology and systems integration that would not otherwise be possible due to the very complex nature of the interacting processes present in large-scale power generators with carbon capture. Such improvements will decrease the cost and improve the performance of CO<sub>2</sub> capture technologies by providing a platform on which different process control schemes can be demonstrated and optimized prior to their implementation in CO<sub>2</sub> capture processes.

# Appendix F: Building Energy Efficiency Consortium Project Fact Sheets

## Integrated Building Design & Operation of Very Low Energy, Low Cost Buildings

Real-time Monitoring and Energy Database .....	F-3
Methods and Tools to Achieve Integrated Building Design* .....	New Project*
Building Performance Simulation.....	F-5
Modeling Behavior* .....	New Project*
Building Energy Analysis, Comparison and Benchmarking .....	F-7

## Building Envelope

Complex Glazing Materials and Shading Systems .....	F-9
Insulation Materials and Systems.....	F-11
Liquid Flashing to Air Seal Windows, Doors and Piping Penetrations* .....	New Project*
Cool Roofs and Urban Heat Islands.....	F-13
Building Natural Ventilation and Cooling Technology Research .....	F-14

## Building Equipment

Dehumidifier Devices*.....	New Project*
Advanced Lighting Controls* .....	New Project*
Evaporative-cooler Chiller*.....	New Project*

## Renewable Energy Utilization

Advanced Ground Source Heat Pump Technology .....	F-16
Building Integrated PV and Microgrids for Low Energy Buildings*.....	New Project*
New and Renewable Energy Technologies .....	F-18
Distributed Energy Supply System Integration .....	F-20

## Whole Building

Energy Systems and Technology* .....	New Project*
Commissioning, Operation, Real Time Monitoring and Evaluation* .....	New Project*

## Operation, Management, Market Promotion and Research

Research on Very Low Energy Building Operations and Management Methods* .....	New Project*
Building Energy Commercialization and Market Research .....	F-21

\* Indicates new projects for year 3 of CERC BEE; fact sheets from year 2 are not available for these recently established projects.



## Research Topics

BEE has developed a collaborative research agenda organized into six research topics (thrust area) as outlined below. Each thrust area saw notable technology developments in year 2 of CERC. Research and accomplishments at the project level are provided in the next section.

*A. Integrated Building Design & Operation of Very Low Energy, Low Cost Buildings:* Provide a rich foundation to support prioritization of energy savings opportunities from buildings. Research in this topic area are focusing on new scientific methods for collecting data and modeling energy consumption that will guide development of high-impact energy efficiency technologies. Key accomplishments in 2012-2013 include:

- Developed and released an on-line comparative energy benchmarking tool
- Expanded use of measured data from real-time monitoring
- Integrated behavioral impacts into simulation models

*B. Building Envelope:* Develop new building materials and related control and integration systems. Research in this area improves understanding and strategies for ventilation, comfort systems, and cool roofs. Accomplishments in the past year include:

- Developed “cool roof” provisions for Chinese national BEE standards
- Designed new fenestration materials and systems
- Tested high efficiency shading and insulated window systems

*C. Building Equipment:* Research and demonstrate the adaptability of advanced building equipment technologies. Research in this area includes new lighting system design and control and improvements to the performance and market penetration of climate control (heating, ventilation, and cooling) technologies. Research includes integrating building equipment with control systems and metering equipment and optimizing management software. Major accomplishments in 2012-2013 include:

- Built integrated control strategies
- Developed advanced algorithms and demonstration programs for lighting
- Produced new advanced evaporative cooling systems

*D. Renewable Energy Utilization:* Research and demonstrate technological adaptability in applying new and renewable energy to buildings. This research area includes integration of geothermal, solar, and wind energy systems, among others, to convert buildings from energy consumers to net energy suppliers. Recent accomplishments include:

- Authored a cloud tool for distributed energy technologies based on load and real time pricing
- Evaluated renewable energy systems
- Designed new ground source heat exchangers

*E. Whole Building:* Research and demonstrate integrated building energy technologies. Research in this area includes analyzing building energy use in the United States and China to improve building integration and optimize the use of energy-efficient and low-carbon energy supply technologies. Major accomplishments in 2012-2013 include:

- Modeled real time strategies for cost and peak load reduction
- Conducted comparative research on energy use of high efficiency buildings in the United States and China

*F. Operation, Management, Market Promotion and Research:* Evaluate standards, certification, codes and labels, and other policy mechanisms to establish a knowledge base from which to make effective decisions. Key accomplishments in 2012-2013 include:

- Developed methodologies for energy cap-and-trade system in buildings and a quota system for public buildings
- Drafted policy recommendations to promote energy efficiency, renewable energy, and green buildings

## Monitoring and Simulation of Building Energy Consumption

## Real-Time Monitoring and Energy Database

Joint Project

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• Lawrence Berkeley National Laboratory</li> <li>• Oak Ridge National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>• Tsinghua University</li> <li>• Persagy</li> </ul>

*Research Objective*

The objectives of the project are to develop a standard methodology for building energy data definition, collection, presentation, and analysis; apply the developed method to a standardized energy monitoring platform, including hardware and software, to collect and analyze building energy use data; and compile off-line statistical data and online real-time data in both China and the United States for a full understanding of the current status of building energy use.

*Technical Approach*

- Compare existing energy monitoring systems
- Develop a standard data model to describe energy use in buildings
- Develop three-level data analysis methods: energy profiling, benchmarking, and diagnostics
- Select a few buildings in the United States and China to collect three types of data: energy use, system and equipment operating conditions, and indoor and outdoor environmental conditions
- Analyze the collected building data to quantify building performance, understand the drivers to discrepancies, and identify potential energy-savings measures

*Recent Progress*

- Identified the need for a standard data model and platform to collect, process, analyze, and exchange building performance data due to different definitions of energy use and boundary, difficulty in exchanging data, and a lack of current standards
- Compared energy monitoring systems to identify gaps, including iSagy, Pulse Energy, SkySpark, sMap, EPP, ION, and Metasys
- Developed a standard data model to represent energy use in buildings (International Organization for Standardization [ISO] standard 12655 and a Chinese national standard)
- Determined that buildings in the United States and China are very different in design, operation, maintenance, and occupant behavior. U.S. buildings have more stringent comfort standards regarding temperature,

ventilation, lighting, and hot-water use and therefore higher internal loads and operating hours. Chinese buildings having higher lighting energy use; seasonal heating, ventilation, and air conditioning (HVAC) operation; more operators; more use of natural ventilation; less outdoor ventilation air; and a wider range of comfort temperature

- Completed data collection for six office buildings: one on the University of California, Merced campus; one in Sacramento; one in Berkeley; one on the George Tech campus; and two in Beijing
- Compiled a source book of 10 selected buildings in the United States and China containing detailed descriptions of the buildings, data points, and monitoring systems, as well as an energy analysis of each building and an energy benchmarking among all of the buildings
- Recognized the limited availability of quality data, particularly with long periods of time-interval data, and the general lack of value for good data and large data sets
- Held a seminar at Lawrence Berkeley National Laboratory to present research findings and seek feedback
- Prepared deliverables for the second year of research

*Expected Outcomes*

- A significant contribution to a standard data model to represent energy use in buildings (ISO standard 12655 and a Chinese national standard)
- A building energy database, with detailed energy end use at 1-hour or 15-minute time intervals, of six office buildings—four in the United States and two in China. The database is available to the public and is a valuable resource for building research
- Methods in data analysis of building performance developed and used for the five buildings with adequate data, including energy benchmarking, profiling (daily, weekly, monthly), and diagnostics
- Recommendations for energy efficiency measures for building retrofit in both the



Figure 1. International Organization for Standardization (ISO) Standard 12655 – Energy Use Data Model.

United States and China. U.S. buildings show more potential savings by reducing operation time, reducing plug-loads, expanding comfort temperature range, and turning off lights or equipment when not in use; while Chinese buildings can save energy by increasing lighting system efficiency and improving envelope insulation and HVAC equipment efficiency

- Numerous publications—researchers have submitted an article that is under review for Building Research and Information, are preparing two journal articles for Applied Energy, and have published four conference papers

Energy Monitoring Systems	Technical features												Analysis features												Fault detection		
	Including hardware for acquisition	Automatic data acquisition	Manual data entry	Automatic data processing	Platform independent	CSV-Import	CSV-Export	Interfaces to BMS	Automatic chart generation	Interactive charts	Stand-alone software	Web frontend	Interpolation if arbitrary measure intervals	Virtual sensors	Definition of any reference values	Comfort analysis	Statistical analysis	Real-time diagnosis	Climate correction	Report system	Tools for benchmarking	Prediction of energy savings	Prediction of cost savings	Analyze building subsystems	Data integrity validation	Check by value ranges	Email notification
iSagy																											
Pulse Energy																											
EPP																											
SkySpark																											
sMAP																											
ION																											

Figure 2. Comparison of building energy monitoring systems.

## Monitoring and Simulation of Building Energy Consumption

## Building Performance Simulation

Joint Project

U.S. Research Team Lead	China Research Team Lead
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*Research Objective*

This project aims to improve and expand the use of building simulation to support the design and operation of low-energy buildings through better understanding and predicting of the energy performance of buildings. The specific research objectives are the following:

- Use and improve building simulation to better understand energy use data of buildings in China and the United States
- Understand and identify key driving forces behind the energy performance of buildings by developing new methods to describe and model these factors
- Evaluate and compare the capabilities of DOE-2.1E, Designer's Simulation Toolkit (DeST), and EnergyPlus to better understand their strengths and weaknesses, which will support their use for energy code development and code compliance in China

*Technical Approach*

- Perform sensitivity and scenario analyses to quantify the relative impact of the six driving factors of the energy performance of buildings
- Identify the key energy-related practices of operation and maintenance, and evaluate their impact on building performance
- Develop methods to describe occupant energy behavior in buildings based on measured and survey data
- Develop algorithms to model occupant behavior and evaluate its impact on building energy use
- Compare DOE-2.1E, DeST, and EnergyPlus to evaluate their capabilities and limitations and recommend their use in energy modeling

*Recent Progress*

- Completed a series of sensitivity and scenario analyses of weather, building operation, maintenance, and occupant behavior. These factors have a significant influence on building energy use and should be correctly considered in evaluating energy efficiency measures during building design and operation

- Held two public workshops in Hong Kong and Shanghai to present research findings and seek feedback from the academic, research, and industrial communities
- Prepared and submitted six journal articles

*Expected Outcomes*

- Improved use of simulation to better understand and evaluate key drivers of building performance
- Identification of new features of EnergyPlus and DeST to be able to model operation faults and maintenance issues. A software module of occupant behavior is under development to co-simulate with EnergyPlus, DeST, etc.

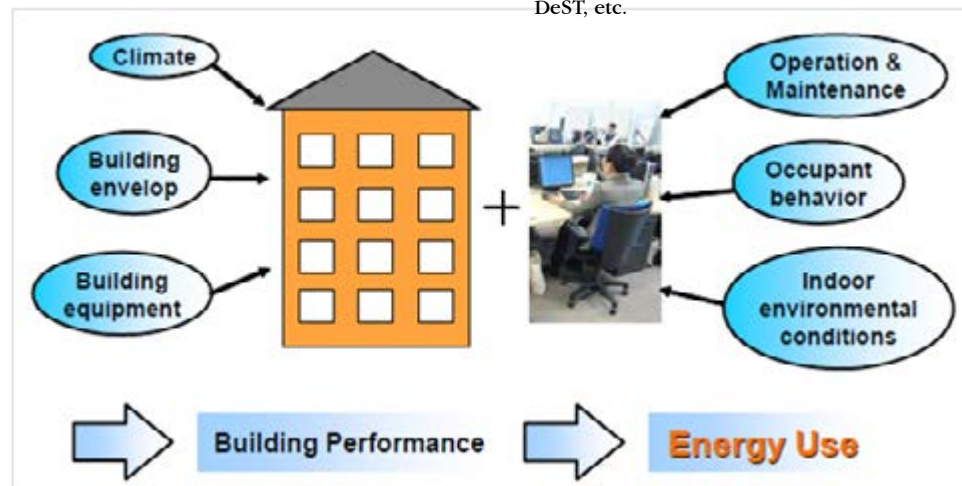


Figure 1. Six driving factors of the energy performance of buildings.

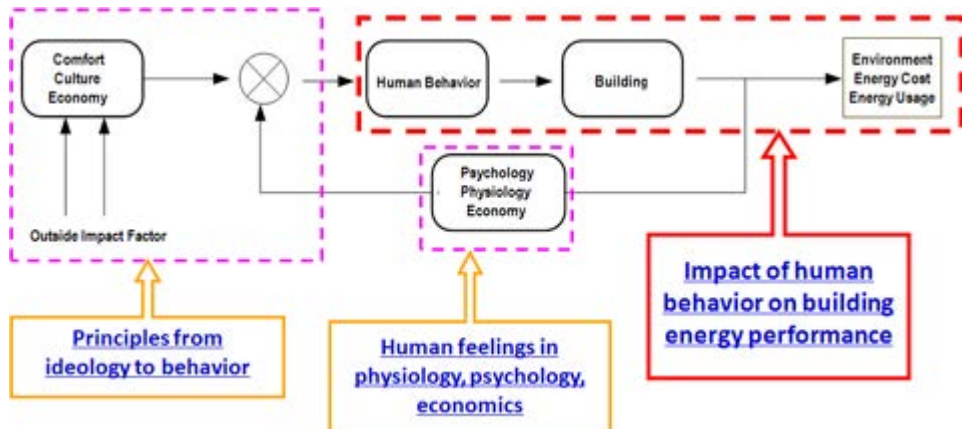


Figure 2. Human behavior and energy use in buildings.



- Increased understanding and reduced uncertainty in using simulation to predict actual building energy performance by taking into account the uncertainty of the key driving factors
- Research on standard simulation input patterns and default settings for codes, evaluation, etc.
- New methods to describe and model occupant behavior in buildings
- A systematic approach to compare building energy modeling programs
- Publication of six articles in Journal of Building Simulation, eight conference papers, and six technical reports (including two Lawrence Berkeley National Laboratory technical reports). These publications describe methods and results to evaluate the impact of key driving factors on energy use in buildings, and to compare and evaluate building energy modeling programs

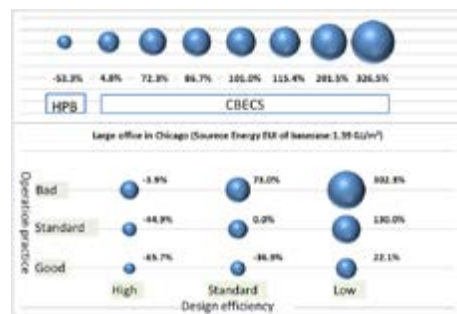


Figure 3. Impact of design and operation on the energy use of buildings.

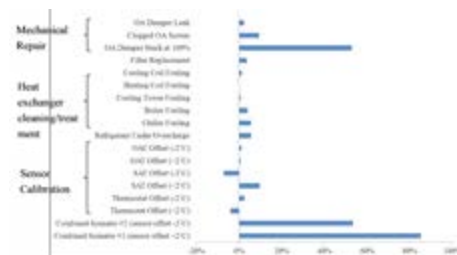


Figure 5. Impact of HVAC maintenance on the energy use of buildings.

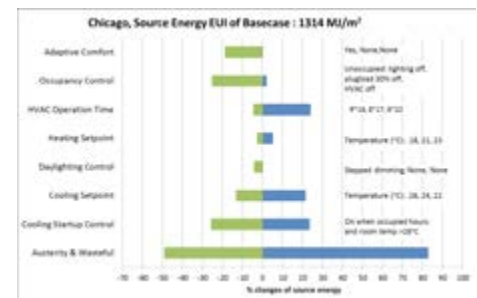


Figure 4. Impact of occupant behavior on the energy use of private offices.

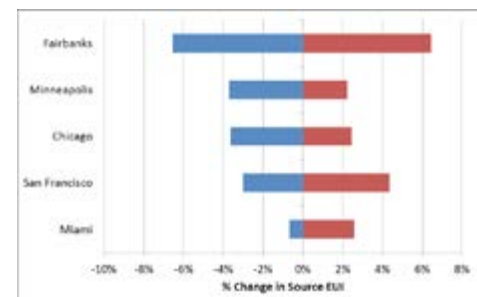


Figure 6. Impact of weather on the energy use of buildings.

## Monitoring and Simulation of Building Energy Consumption

## Building Energy Analysis, Comparison and Benchmarking

Joint Project

U.S. Research Team Lead	China Research Team Lead
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*Research Objective*

The primary objectives of this project are the following:

- Develop market-oriented, practical systems for benchmarking building energy performance in hotels and commercial offices in China
- Develop an understanding of the key drivers for top energy performance in hotel and commercial office buildings in China and an understanding of how those compare to key performance drivers in the United States
- Gain an initial understanding of how building energy performance in China compares to building energy performance in the United States
- Identify lessons and best practices that can be shared between China and the United States to improve building energy performance in both countries
- As a secondary objective, researchers will conduct analyses of large homogenous portfolios of building data to identify the factors that cause common energy performance variations across those data sets.

*Technical Approach*

- Use nationally representative data sets (when available)
- Compare energy performance in terms of source energy
- Perform multiple regression analyses to find the combination of statistically significant operating characteristics that explain the greatest amount of variance in building source energy use
- Use the nationally representative data set to determine the distribution of energy performance across the entire population of hotels. A table is created and the benchmark rating is based on the ratio of actual energy consumption to that predicted by the regression analysis.

*Recent Progress*

- Completed a Web-based benchmarking tool for hotels that is housed at a permanent sustainable institute in China—the China Academy of Building Research
- Developed an Excel-based prototype benchmarking tool for commercial offices that automatically normalizes for the key drivers of energy use in Chinese commercial offices (size, location, operating hours, etc.) so office energy performance can be fairly compared
- Identified refreshable online and survey data sources and processes for ongoing maintenance and updates to the tools based on incoming data and feedback on tool functionality
- Determined the statistically significant operating characteristics that explain the greatest variance in energy usage by conducting multiple regression analyses on hundreds of Chinese commercial offices and hotels. Made comparisons to the statistically significant drivers of building energy use as identified by the U.S. ENERGY STAR program to identify similarities and differences
- Developed an initial understanding of how hotel and commercial office building energy performance compares in China and the United States by performing simple energy usage per square meter benchmarking for large building data sets in China

*Expected Outcomes*

- Significant potential energy and CO<sub>2</sub> emission reductions over the short and long terms as a result of the availability of comparative energy benchmarking tools for hotels and commercial office buildings in China (as detailed in Table 1)
- A marked increase in sales of energy-saving technologies and building equipment due to the availability of comparative building benchmarking tools and more buildings obtaining a practical understanding of their energy performance and need for improvement. As the leading suppliers of



Figure 1. The hotel benchmarking tool is complete and available online at <http://www.cabr-cecc.com/>.

green building technologies globally, U.S. companies stand to gain a substantial market share of these equipment and technology sales in China. If approximately one-third of all buildings benchmarked invested in advanced lighting; heating, ventilation, and air-conditioning systems; and other equipment and technologies, U.S. companies could generate substantial additional sales and revenue (as detailed in Table 2)

Time Period	Total Floor Area Benchmarked (Sq M)	GHG Emission Reduction (MtCO <sub>2</sub> e)	Equivalent Trees Planted
Short-term: 2015-2017	58,800,000	1,899,595	48,707,564
Long-term: 2015-2025	342,000,000	38,642,440	990,831,795

Table 1. China Energy and CO<sub>2</sub> Impact

Time Period	Total Square Meters Investing in Technology	Estimated Retrofit Cost Per Square Meter (USD)	Total Sales (USD)
Short-term: 2015-2017	17,640,000	\$82.93	\$1,462,858,602
Long-term: 2015-2025	102,600,000	\$82.93	\$8,508,463,295

Table 2. Projected Revenue from Sale of U.S. Green Building Technologies in China

## Building Envelope Systems

## Complex Glazing Materials and Shading Systems

Joint Project

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U.S. Partners	China Partners	
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*Research Objective*

The primary objectives of this project are the following:

- Identify and develop the methods needed to characterize, compare, and evaluate the energy use and comfort performance of window and shading technologies
- Identify, develop, and evaluate the window and shading technologies needed to attain energy efficiency goals for residential and commercial buildings in a diverse set of climates in the United States and China

*Technical Approach*

- Define and share the current methods for characterizing and modeling the energy efficiency performance of window systems
- Use simulation tools, laboratory and full-scale field tests, and demonstrations in occupied buildings to quantify and improve the energy efficiency, comfort, and indoor environmental quality impacts of advanced emerging technologies
- Promote the use of identified energy-efficient solutions through application and technical guidelines

*Recent Progress*

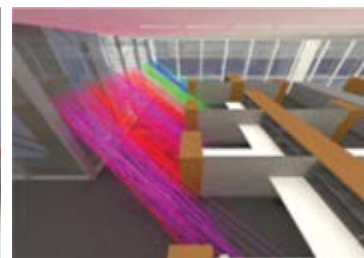
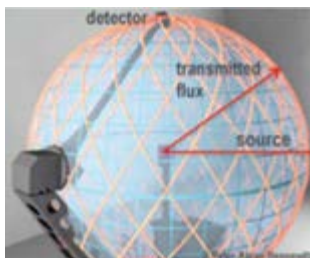
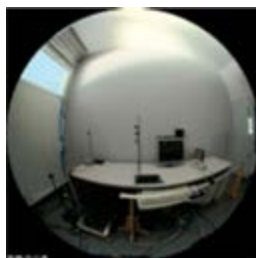
- Completed a technical assessment of the energy-savings potential of fenestration-related energy efficiency measures that are likely to produce significant reductions in energy use in commercial buildings in China. Compared to the energy efficiency code in effect in China (GB 50189-2005), conventional low-emittance windows with exterior operable shading were able to achieve up to 66% savings in perimeter zone heating, ventilation, and air conditioning (HVAC) electricity consumption; 5% savings in district heating energy in the cold climate of Beijing; and up to 42% savings in HVAC electricity consumption in the hot/cold climate of Shanghai. Highly

insulating windows also had a significant effect on reducing energy use and were recommended for new construction. Results were summarized in an article submitted to the Building Research & Information journal

- Continued to develop the simulation tools needed to model the daylighting and window heat gain performance of optically complex fenestration systems (CFSs) because shading attachments are likely to be a near-term, low-cost solution for retrofit and new construction in both the United States and China. Collaborative activity focused on understanding the methods used to introduce standardized calculation procedures to the Chinese codes and standards process with the goal of promoting international harmonization of methods to evaluate shading technologies. Year 3 activities will focus on extending Year 2 work by encouraging the adoption of standard calculation procedures for evaluating CFSs so that products can be compared in both the United States and China. CFSs scatter light in a non-specular manner. A scanning goniophotometer can measure the angular-dependent reflected

and transmitted radiation of CFS materials and systems, and these data can then be used in simulation tools such as Window 7, Radiance, and EnergyPlus to determine annual energy performance and comfort impacts

- Initiated discussions with the Saint-Gobain Research Center in Shanghai regarding research objectives, approach, technical details of construction, instrumentation, and monitoring related to conducting a monitoring demonstration of dynamic electrochromic windows in its new center. The Saint-Gobain Research Center in Shanghai agreed to permit the monitored demonstration in order to better understand the technology and its impacts on energy use and occupant comfort. Dynamic, automated window systems are likely to produce the ultra-low energy savings that both the United States and China are striving to attain. The three-story research center is under construction, and the electrochromic windows are expected to be installed in summer 2013



Figures 1–3. (1) Sunlight-redirecting film in a full-scale test bed office, (2) a scanning goniophotometer, and (3) an image from the Radiance simulation tool.



### *Expected Outcomes*

- Improved prototype emerging technologies based on quantitative feedback from laboratory and field studies in collaboration with industry
- Increased confidence of suppliers and the architectural-engineering community in specifying the investigated emerging technologies in the United States and China based on more accurate, validated simulation tools at the early stages of design and third-party measured data of the technology in real buildings. Accelerated market adoption of low-energy façade technologies



Figure 4. Rendering of the new addition to the Saint-Gobain Research Center in Shanghai where electrochromic windows will be evaluated in two side-by-side conference rooms.

## Building Envelope Systems

## Insulation Materials and Systems

Joint Project

U.S. Research Team Lead	China Research Team Lead	
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U.S. Partners	China Partners	
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*Research Objective*

This project will identify and investigate candidate high-performance, fire-resistant building insulation technologies that meet the goal of building code compliance for exterior wall applications in green buildings in multiple climate zones.

*Technical Approach*

- Investigate candidate building insulation materials and systems that meet the goals of fire safety, cost effectiveness, and performance; noting that the target goals may vary greatly in different economies and locations
  - This research will cover areas of thermal performance, including the changes that may occur over time due to exposure to the elements and moisture
- Investigate system issues that can affect performance, such as attachment systems and thermal breaks
  - Make direct laboratory and field measurements in some cases
- Use simulations to support the research and to explore the efficacy of systems in multiple climates where necessary
- Make maximum use of existing experimental data to increase the efficiency of the research effort in all cases
- Perform a market analysis to identify barriers and gaps preventing the widespread adoption of the best technologies in China
  - Identify best practices and lessons learned in both China and the United States based on this survey

*Recent Progress*

- Conducted an initial review and comparison of U.S. and Chinese building codes and standards according to climate and building type. American Society of Heating, Refrigerating and Air Conditioning Engineers (ASHRAE) 90.1 and the International Energy Conservation Code (IECC) are the primary building codes implemented in the United

States. Both residential and public building code requirements in the United States and China were compared on the basis of similar climate zones (heating/cooling degree days), revealing some interesting features. For some cases, such as public building windows and residential walls in certain climates types, the U.S. and Chinese building code requirements are comparable. In other cases, the U.S. code requirements are usually more stringent. Comparison of the required thermal transmittance (U-values) of public building envelope components are presented in Figures 1–3

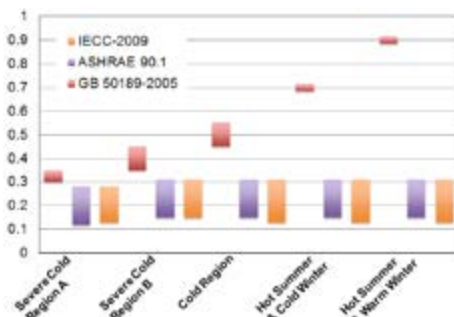


Figure 1. Public building roof U values (W/m²·K) for multiple and similar climate zones in the United States and China.

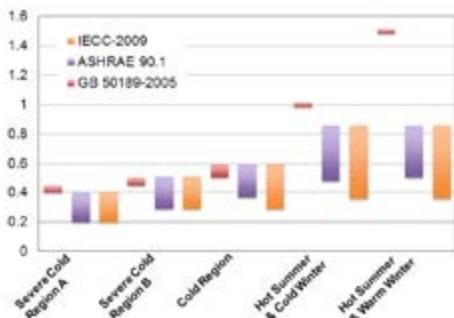


Figure 2. Public building wall U values (W/m²·K) for multiple and similar climate zones in the United States and China.

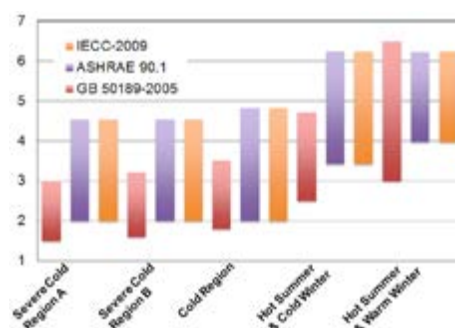


Figure 3. Public building window U values (W/m²·K) for multiple and similar climate zones in the United States and China.

- Reviewed retrofit and weatherization strategies for single-family and multifamily residential buildings from a building envelope perspective. Researchers compiled a list of prioritized weatherization measures for site-built homes from a local weatherization field standards document in the United States that included both mandatory and recommended measures. They also reviewed and described various case studies that utilized both interior and exterior envelope insulation retrofit, highlighting moisture-related challenges encountered in interior envelope insulation retrofits, especially in cold climates, and possible remediation measures
- Reviewed wall insulation systems in Europe, the United States, and China. The review focused on the development and current status of exterior wall insulation systems. Exterior wall insulation has many advantages over interior insulation and is currently the leading wall insulation technology in China. Exterior insulation systems are based on either foam or rock wool insulation. In the United States and Europe, foam insulation is more commonly used in low-rise buildings and rock wool is used in tall buildings. Recently, vacuum insulation panels have been evaluated for exterior insulation systems, but they have yet to achieve wide acceptance

- Reviewed the U.S. fire safety codes and flammability standards for insulation materials and systems. The main fire code in the United States is the International Fire Code (IFC, 2009) from the International Code Council, Inc., but based on specific conditions, individual states enforce additional fire safety codes. In addition to building codes, insulation materials and building envelope assemblies are also tested and rated according to different standard test methods from ASTM International, Underwriters Laboratories, and the National Fire Protection Association

#### *Expected Outcomes*

- The initial research results were summarized in an August 2012 joint Oak Ridge National Laboratory-China Academy of Building Research wrap-up report that focused on the review of building codes, insulation systems, weatherization methods, and fire safety codes in the United States as well as a comparison with relevant Chinese codes and standards
- The insulation materials and systems portion of the project was cancelled after Year 1

## Building Envelope Systems

## Cool Roofs &amp; Urban Heat Islands

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>Oak Ridge National Laboratory</li> <li>Dow Chemical</li> </ul>	<ul style="list-style-type: none"> <li>Guangdong Provincial Academy of Building Research</li> <li>China Icepower Energy Technology Co., Ltd</li> </ul>

*Research Objective*

This project will quantify the potential energy and environmental benefits of cool roofs in China—especially carbon reduction—and help develop the infrastructure (including policies and rating systems) needed to promote the appropriate use of cool roofs. It will also develop stay-clean white roofing products for the China and U.S. markets.

*Technical Approach*

This project will investigate how cool roof technology may best be adapted to Chinese climates, urban design, and building practices. In particular, the research team will accomplish the following:

- Understand through technical exchange the state of the art of materials, measurement techniques, and energy efficiency standards for cool roofs
- Quantify for Chinese climates, urban design, and building practices the benefits of cool roofs, such as energy savings, greenhouse gas reductions, urban cooling, improved air quality, and improved human health
- Assess for Chinese climates, urban design, and building practices the advantages and disadvantages of cool roofs when compared to traditional roofs
- Initiate the infrastructure needed to promote the appropriate use of cool roofs in China
- Design (and possibly initiate) a large-scale cool roof/cool pavement demonstration project in China
- Develop superhydrophobic white roof coatings with improved durability and long-term solar reflectance

*Recent Progress*

- Submitted to Building Research & Information an extensive study that simulates and measures the benefits of cool roofs in China and reviews the role of cool roofs in Chinese building energy standards. The study found that cool roofs conserve energy, save money, and reduce emissions in all Chinese climates with hot summers

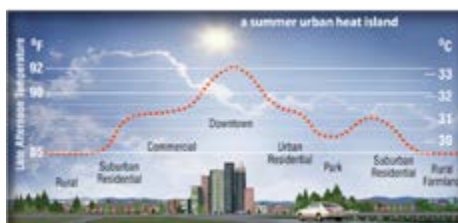


Figure 1. Illustration of the urban heat island effect.

- Hosted day-long cool roof workshops at Lawrence Berkeley National Laboratory (LBNL) and Oak Ridge National Laboratory (ORNL) for 30 members of the Chinese National Building Waterproof Association, which represents Chinese roofing manufacturers. These workshops featured discussions and demonstrations of U.S. and Chinese cool roof science, technology, and infrastructure that helped further the research teams' collaborative relationship
- Executed a three-way cooperative research and development agreement (CRADA) entitled "Development of a Long Life Cycle, Highly Water Resistant, Solar Reflective Retrofit Roof Coating," No. NFE-12-04205, between UT-Battelle (operator of ORNL), the University of California (operator of LBNL), and The Dow Chemical Company, enabling collaborative research to begin on March 12, 2013
- Initiated technical discussions with Dow Chemical Company on March 12 with the goal of jointly developing highly water-repellent and anti-biofouling cool roof coatings as per subtask 9 of project B3 – Cool Roofs & Urban Heat Islands
- Fabricated several samples since March 12 of superhydrophobic silica-based powders for testing and incorporation in latex-based cool roof coatings at Dow

*Expected Outcomes*

- Climate-specific quantification and demonstration of the potential benefits of cool roofs in China, including energy savings, cost savings, and emission reductions



Figure 2. Water drop sitting on top of a circular superhydrophobic surface surrounded by water.

- A model code for cool roof incentives/requirements for local and/or national building energy efficiency standards and greenhouse gas reduction plans in China
- Solar reflectance and other measurement techniques needed to identify and market cool roofing products
- A large-scale cool roof/cool pavement project in China demonstrating both building energy savings and summer urban heat island mitigation
- Development of environmentally friendly, water-based superhydrophobic and anti-biofouling cool roof coatings that will be tested on commercial building roofs both in the United States and China

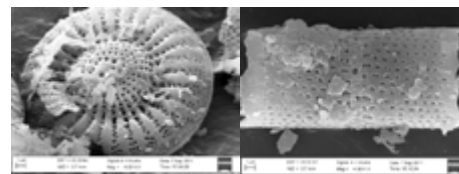


Figure 3. Two types of diatomaceous earth powders used to make extremely water-repellent surfaces.



## Building Envelope Systems

# Building Natural Ventilation and Cooling Technology Research

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
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## Research Objective

This project will determine the potential of natural ventilation to provide comfortable conditions and reduce or eliminate the need for air conditioning over the important climatic zones in China and the United States. Implementing this technology in China, the United States, and other countries, and developing design tools that can be used in new or retrofit designs, will promote the widespread application of this technology for energy efficiency and improved indoor climatic conditions.

## Technical Approach

- Conduct a survey of natural ventilation in the United States and China and consider adaptable ventilation techniques—this will identify methods and systems of cooling by ventilation that are effective in different climate zones
- Conduct an analysis of the impacts of different ventilation systems on the indoor thermal environment
- Use an enhanced edition of Massachusetts Institute of Technology (MIT) design programs using multi-node solutions that include transient thermal mass heat transfer and wind-, buoyancy-, and mechanical-driven flows to design prototype natural ventilation cooling systems that will act as retrofit natural ventilation demonstrations in several existing MIT academic buildings and Chinese demonstrations
- Develop control algorithms for buildings with hybrid natural-mechanical ventilation that maximize energy savings according to building and ventilation configuration
- Develop design and operation guidelines for buildings with hybrid ventilation systems

## Recent Progress

- Completed a final joint research plan
- Improved MIT design software that can be used to analyze buildings with hybrid ventilation systems; this design software is capable of simulating ventilation fans and air conditioning units
- Determined energy savings for the most relevant commercial buildings in 10 important U.S. cities in different climate zones for different ventilation strategies using the U.S. Department of Energy building benchmark
- Started coding of an optimization process for hybrid ventilation systems
- Completed monitoring of a demonstration building in the United States. Completed a report with a methodology, results, and recommendations. Natural ventilation was found to be used below its optimum potential. Use of a ventilation fan was found to be inefficient
- Identified five potential demonstration buildings in different weather regions in China, including a new development
- Started an analysis of radiation processes on thermal stratification in buildings to better determine comfort conditions in naturally ventilated buildings
- Completed a survey of natural ventilation technology applications in China and the United States. Key findings of the Chinese side were that designers play the most important role in the application of natural ventilation. While the importance of this technology is acknowledged, its application is limited due to a lack of appropriate simulation programs. Key meteorological data for application of natural ventilation technology require local measurements within specific urban areas where it will be applied

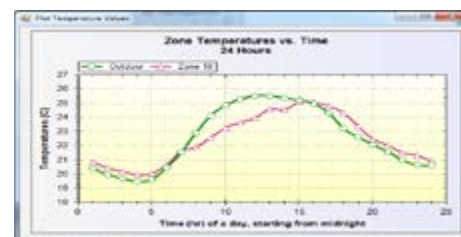


Figure 1. Sample results for night cooling obtained using CoolVent.

## Expected Outcomes

- Identification and design of natural ventilation demonstration buildings in relevant areas in the United States and China
- Development of application, design, and operation guidelines for hybrid natural-mechanical ventilation techniques that are adaptable for different building types and climate zones
- An improved design program that can be used for the following:
  - Determining the characteristics that all successful naturally ventilated buildings share, and compiling them in design and operation guidelines for hybrid natural-mechanical ventilation systems
  - Evaluating the performance of demonstration buildings in relevant climate zones in both China and the United States

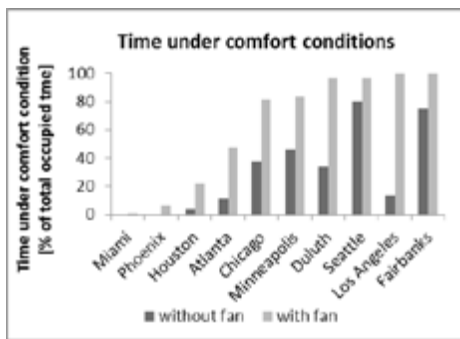


Figure 2. Hybrid ventilation significantly improves comfort conditions in a typical strip mall building. The energy consumption of a ventilation fan is small.

- Determining energy savings for different weather regions, building types, and ventilation configurations in the United States and China
- Assisting the Shenzhen Institute of Building Research in the evaluation of a new construction project in China
- Development of control algorithms for hybrid ventilated buildings that can be used as part of a window heating, ventilation, and air conditioning control system
- Improved thermal stratification models that better predict comfort conditions in naturally ventilated buildings

## Renewable Energy Utilization

## Advanced Ground Source Heat Pump Technology

Joint Project

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>Oak Ridge National Laboratory</li> <li>ClimateMaster</li> </ul>	<ul style="list-style-type: none"> <li>Chongqing University</li> <li>Tianjin University</li> <li>Tongji University</li> <li>ENN Group Co., Ltd</li> <li>Zhuhai Singyes Green Building Technology Co., Ltd</li> <li>Suntech Power Holdings Co., Ltd</li> <li>Zhejiang Shield Equipment Company Limited</li> <li>Ever Source Science and Technology Development Co., Ltd</li> <li>Himin Solar Energy Group Co., Ltd</li> <li>Jiangsu Joint Hot and Cold Energy Saving Equipment Co., Ltd</li> <li>Landsea Group Co., Ltd</li> <li>Futian Air Conditioning Equipment Co., Ltd</li> </ul>

*Research Objective*

This project will compare the status and trends of ground source heat pump (GSHP) technology in both China and the United States to identify differences and areas in which each country can learn from each other to enable wider adoption of the technology. Through extensive data collection and analysis, researchers will assess the cost and benefits of GSHP applications in various conditions in both countries. Researchers will also evaluate the potential of various emerging GSHP technologies in reducing the cost and/or improving the performance of GSHP systems. They will also develop optimal controls to maximize the operational efficiency of GSHP systems.

*Technical Approach*

- Investigate the applications of GSHP technology (including the shallow surface ground source heat pump, the surface water and wastewater source heat pump, and the standing column well ground water heat pump) in both China and the United States to understand the status and trends of the technology; its applications, market, and related policies; the barriers preventing further development of the technology; and solutions to overcome the barriers
- Develop methodologies and tools to evaluate the suitability of GSHP applications at various conditions based on performance data collected from GSHP systems installed in both China and the United States
- Evaluate emerging technologies or products in both countries, including system configurations, ground coupling technologies, heat pump equipment, monitoring and control systems, and design software that may help break the cost barrier and/or further improve the efficiency of GSHP systems

- Identify and implement optimal controls for GSHP equipment and distributed GSHP systems
- Initiate and design a demonstration project in China to demonstrate advancements in GSHP technology

*Recent Progress*

- Identified alternative ground heat exchangers (GHXs) that require 21%–36% less drilling depth compared with conventional GHXs while retaining the same performance and completed a technical report of the study (Field Test and Evaluation of Residential Ground Source Heat Pump Systems Using Emerging Ground Coupling Technologies, ORNL/TM-2013/39)
- Submitted to Building Research & Information a comprehensive study that compares the major differences in GSHP applications in China and the United States. These differences include the presence of mostly closed-loop GHXs in the United States versus groundwater, surface water, and wastewater GHXs in China; the presence of mostly small and mid-size buildings in the United States versus large buildings in China; the presence of mostly decentralized systems in the United States versus centralized systems in China; and that high initial cost is the primary barrier to consumers in the United States versus a lack of standards governing the quality of equipment, design, installation, and operation of GSHP systems as the main barrier in China
- Conducted an extensive parametric study to identify key parameters that are most influential to the economical viability of GSHP applications at various climate conditions in the United States

- Developed a data collection protocol, a set of performance metrics, and a procedure for evaluating the cost effectiveness of GSHP systems
- Performed a preliminary analysis of the performance data of two heating, ventilation, and air conditioning systems installed at the American Society of Heating, Refrigerating and Air Conditioning Engineers' headquarters—a variable refrigerant flow system conditioning the first floor and a distributed GSHP system conditioning the nearly identical second floor
- Surveyed available geological information required in the design and installation of vertical bore GHXs
- Initiated a cooperative research and development agreement (CRADA) entitled "Smart Tank and Smart Control for Ground Source Heat Pump Systems" between UT-Battelle (operator of Oak Ridge National Laboratory [ORNL]) and ClimateMaster that is currently under review by both parties
- Hosted a visit at ORNL by a delegation from Broad Homes Industrial, a large home builder in China, and ClimateMaster to discuss the potential demonstration of the advanced GSHP technology in China

*Expected Outcomes*

- A comprehensive review of GSHP applications in both China and the United States
- A performance evaluation of various GSHP systems in both China and the United States
- Cost reduction and performance-neutral alternative vertical bore GHXs
- Optimized controls for GSHP equipment and distributed GSHP systems

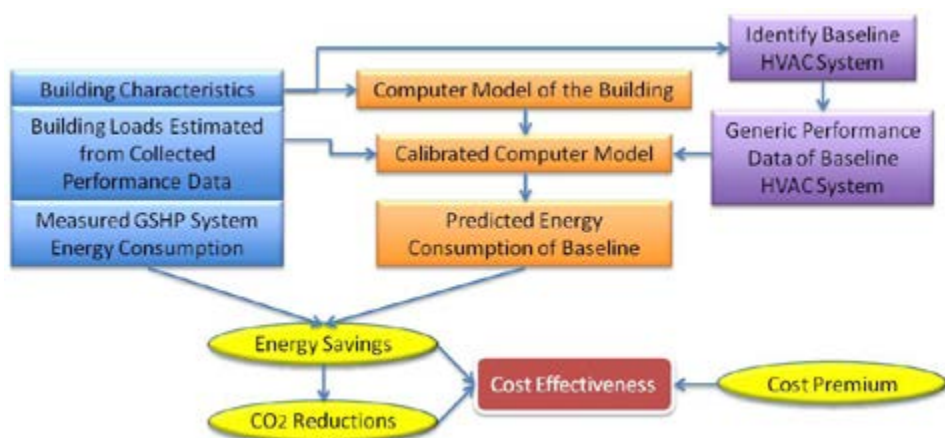


Figure 1. Flow chart of the procedure for evaluating the cost effectiveness of a GSHP application.

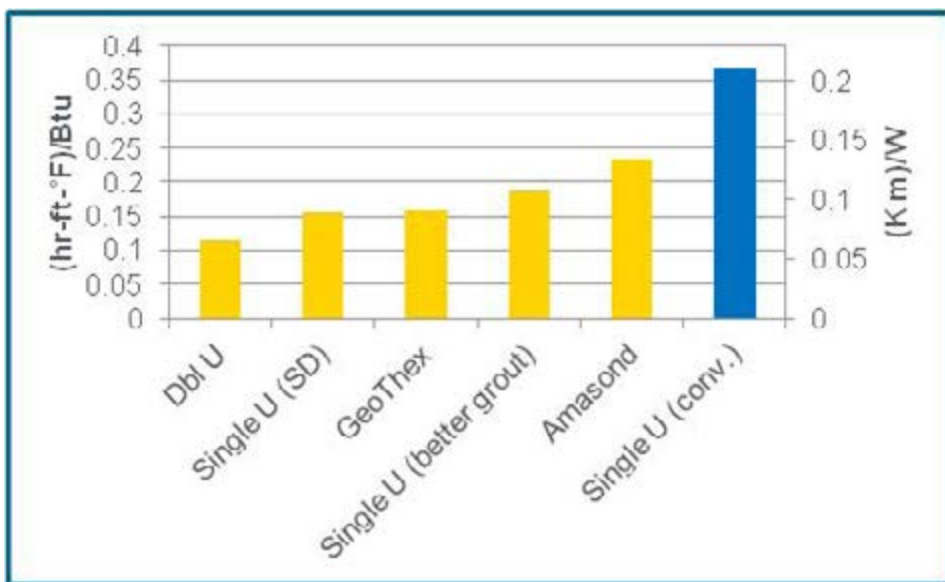


Figure 2. Comparison of borehole thermal resistances between the alternative GHXs and the conventional single U-tube GHX.



## Renewable Energy Utilization

## New and Renewable Energy Technologies

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>Lawrence Berkeley National Laboratory</li> </ul>	

*Research Objective*

This project aims to develop a platform to evaluate the adaptability and optimize the operation of building energy systems involving renewable energy, especially building-scale solar; this work also involves building a related database and creating optimization tools.

*Technical Approach*

- Create an open-access website (Low Energy Building Optimization Web Service [WebOpt])—together with efforts under task D/E.2—based on Lawrence Berkeley National Laboratory's (LBNL's) Distributed Energy Resources Customer Adoption Model (DER-CAM). DER-CAM provides pure analytic optimization, minimizing either the cost or carbon footprint of providing building energy services. The trade-off between the two objectives is often of great interest
- Integrate the database and tools to improve the platform and apply it to case studies. Buildings with high-solar-content energy supply will be studied in detail
- Conduct regional studies of renewables potential, especially involving building-scale solar
- Model buildings with high-solar-content energy systems and develop approaches to optimizing their operations. It is important to note that DER-CAM delivers both equipment selection and optimal operating schedules. Solar cooling systems are of particular interest because of the high cooling loads in parts of both the United States and China, and the low market penetration of absorption cooling. LBNL is already working closely with the University of New Mexico on controlling a campus building with solar thermal cooling, and a sister site has been identified in China



Figure 1. Basic DER-CAM data flow, with key inputs to the left, outputs to the right, and objectives in the center.

*Recent Progress*

- Completed the Chinese interface version of WebOpt, as described in task D/E.2
- Completed analysis of the Shanghai shopping mall distributed energy optimization. This example building has been extensively studied in the literature and has been a powerful pedagogical tool. The mall's electricity requirements are met by a complex combination of equipment—a large combined heat and power (CHP) system consisting of natural-gas-fired gensets with heat recovery was installed. WebOpt displays the electricity requirement that is offset by the waste-heat-driven absorption chiller. This is one of the most valuable results that WebOpt can deliver. This kind of result can never be found by simple methods because of the complex trade-offs between the electrical and heat sides of the building's energy system. As a result, CHP is shown to be a promising technology for eastern China as well as for the United States. Cooling can be attractive where natural gas is available as an environmentally acceptable urban fuel at reasonable cost, electricity is reasonably expensive, and cooling loads are high-waste-heat driven. This is important for solar

thermal penetration because solar assistance to the heat system can be economically attractive in a way that will rarely be discovered with simple methods

- Developed a heat pump module and added it to the WebOpt version. This was a significant improvement of great interest to both the United States and China, as well as to users in Europe. DER-CAM is an analytic model that has significant speed and other advantages; however, the addition of certain equipment, such as devices that use multiple fuels or deliver multiple services, involves significant effort
- Conducted multiple training sessions in China and organized regular conference calls
- Identified and visited buildings with high solar thermal potential

*Expected Outcomes*

- An open-access WebOpt service that is widely available and delivers results that take into account building service requirements, available distributed energy resource technologies, possible efficiency and passive measures, the cost of electricity/natural gas and other fuels under complex tariffs, and available local energy harvesting opportunities

- Low-energy or low-carbon building solutions will be returned in the form of an optimal technology installation choice and optimal operation schedules, cost analyses, scenario comparisons, etc.
- The service will simulate whole building and ultimately multibuilding environments in the United States, China, and elsewhere
- Extended capabilities that allow actual building operation using a Software-as-a-Service (SaaS) model, which greatly simplifies licensing, training, etc.

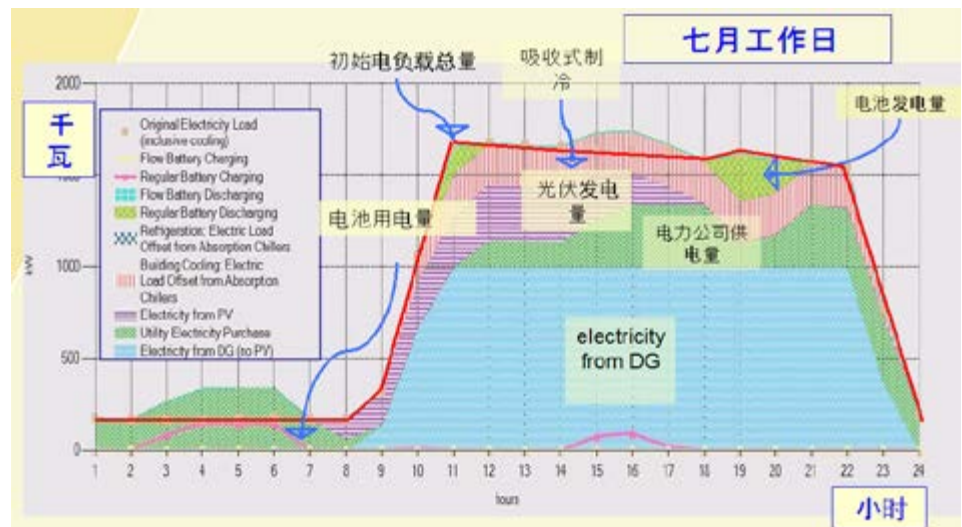


Figure 2. WebOpt Shanghai shopping mall result screen. The mall's electricity requirement is noted by the red line. The electricity requirement that is offset by the waste-heat-driven absorption chiller is noted by the salmon shading.

## Renewable Energy Utilization

## Distributed Energy Supply System Integration

## Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>Lawrence Berkeley National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>Tianjin University</li> </ul>

*Research Objective*

This project's goal is to create an open-access Web service, the Low Energy Building Optimization Web Service (WebOpt), based on Lawrence Berkeley National Laboratory's (LBNL's) Distributed Energy Resources Customer Adoption Model (DER-CAM). The service will permit optimization of building equipment selection (investment decision making) and actual equipment control for building-scale systems and microgrids (operations decision making).

The project's initial work focuses on single building optimization and investment decision making. The longer-term objective is to develop capabilities in the United States and China for building operations decision making. This system would deliver a 2–7-days-ahead optimal operating schedule for controllable building equipment that can be implemented in existing building systems.

*Technical Approach*

- Make the WebOpt version of DER-CAM available in China. Investment decision making is a static process and is readily implemented as a Web service. The user can cut and paste data describing the problem at hand, and results are immediately available as text or simple graphic output
- Extend the existing WebOpt interface to make it more accessible from China and other countries, and demonstrate that working over the Web on an LBNL server is practical. This arrangement significantly reduces implementation and licensing barriers to software deployment
- Use WebOPT to expand on existing DER-CAM capabilities linking to building management/data gathering systems, and expand to focus on conditions in China
- Developed a Chinese language interface. If a user answers an initial question in Chinese, the interface switches to Chinese. The Chinese language version has been very popular and almost all Chinese users choose it. Chinese users now represent about 20% of the more than 200 WebOpt users worldwide
- Conducted training in China and assisted Tianjin researchers with analysis of several existing buildings they have under study, including Building 26 on the Tianjin campus. This building houses a preeminent microgrid research laboratory and is developing a modern control system. This offers an opportunity to directly control the building from an LBNL server, as a pilot for the new buildings
- LBNL will assist with the design and operation of five new demonstration buildings
- Completed a regional study of the technology potential for 11 Chinese cities,



Figure 1. Global locations of current WebOpt users.

covering commercial and multifamily residential buildings. The study confirmed the importance of tariffs, noting that commercial ones tend to stimulation combined heat and power adoption while residential ones do not

*Expected Outcomes*

- A fully integrated building optimization approach that is available to Chinese researchers. This can assist in design and equipment choice
- Analysis of buildings that will guide researchers toward wise choices of renewable use, storage options, etc.
- Direct control of buildings from a remote server that can improve the operation of the buildings via implementation in building control systems and operating procedures



Figure 3. Control system in Building 26 on the Tianjin campus.



Figure 2. Chinese WebOpt screenshot.



Figure 4. Eleven Chinese cities included in regional study of technology potential.

*Recent Progress*

- Extended the capability to run DER-CAM over the Web from China and other countries. Two new servers have been installed and have greatly increased capability. China is by far the fastest-growing region in terms of number of worldwide users. In addition to faster response, the additional hardware has permitted the introduction of an ongoing database of



## Operation, Management, Market Promotion and Research

# Building Energy Commercialization and Market Research

Joint Project

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## Research Objective

This project will review, compare, and analyze laws, regulations, and incentives designed to promote an increase in building energy efficiency in the United States and China, as well as investigate how to formulate policy recommendations and measures to more effectively promote building energy efficiency in the two countries.

The objective is to provide policy information and recommendations on achieving carbon reduction and energy efficiency goals for existing and new buildings through market and regulatory mechanisms targeted at rating and labeling systems, building energy quota and carbon trading schemes, energy efficiency and renewable energy policies, green buildings, retro-commissioning (RCx), energy service companies, incentives for advanced building technologies, and other strategies.

## Technical Approach

- Study existing policy systems and best practices, such as building rating, labeling, and financial incentives, through a literature review of publications and reports and consultation with building energy policy experts. Collaborate with the Ministry of Housing and Urban-Rural Development (MoHURD) and other local partners through open discussions, workshops, and joint research to gain a deeper understanding of China's building energy efficiency industry and policies
- Use a network of experts, working groups, and peer-to-peer interactions in the format of open discussions and workshops to analyze policy trends and identify programs and policies—such as codes and standards, financial incentives, and educational programs—that are needed and can be influenced
- Compile policy and technical information as well as information on industrial experiences, and promote leading international best practices in areas such as RCx and energy service companies



Figure 1. Participants at a joint workshop on Building Energy Quotas held at the National Resources Defense Council's Beijing office in March 2012.

- Conduct case studies and lay the groundwork for governments to initiate and market pilot projects wherever feasible and desirable. For example, a case study on the integrated design method for high-performance buildings was included in one of the policy research topics

## Recent Progress

### Achievements in the First Project Year

- Completed a report comparing U.S. and Chinese building labeling and rating systems. The report includes a detailed comparison matrix jointly developed with MoHURD—containing 34 categories covering background, policy aspects, technical aspects, and real projects—which greatly facilitates the comparison, analysis, and potential alignment of U.S. and Chinese building rating and labeling systems
- Completed research into methodologies for setting building energy consumption quotas and carbon trading schemes. This research culminated in a comprehensive review of all available and relevant international experiences, from Tokyo to the European Union to California. The National Resources

Defense Council (NRDC) held a successful workshop with MoHURD where researchers explained how value-based energy quotas can face fundamental problems and proposed an alternative approach

- Completed a comprehensive report examining U.S. and Chinese policies on building energy efficiency, green buildings, and renewable energy use in buildings. Through comparisons and discussions with Chinese partners, this joint study of U.S. and Chinese building energy policies and experiences has laid a good foundation for further research collaboration

### Progress in the Second Project Year

- Conducted research and drafted reports on three topics entitled: (1) Role of Incentives in Promoting Advanced Building Technology Development and Application, (2) International Best Practices in Building Retro-Commissioning, and (3) Analysis and Introduction of U.S. Experience in the Energy Service (Energy Service Companies) Industry for the Building Sector. These projects are still in progress and will be complete by the end of June



- NRDC building experts conducted a face-to-face open discussion with MoHURD to introduce New York Building Energy Efficiency Rating and Data Disclosure policies and discuss potential policy improvement in China and future collaboration

#### Expected Outcomes

- A workshop with MoHURD and industrial partners to disseminate the U.S.-China Clean Energy Research Center policy and market research results and to promote energy efficiency and international best practices. This workshop will raise awareness among the Chinese government and other partners about policy gaps and the research team's recommendations
- Final reports on three topics: advanced building technology policies, RCx international best practices, and ESCO experience and policies

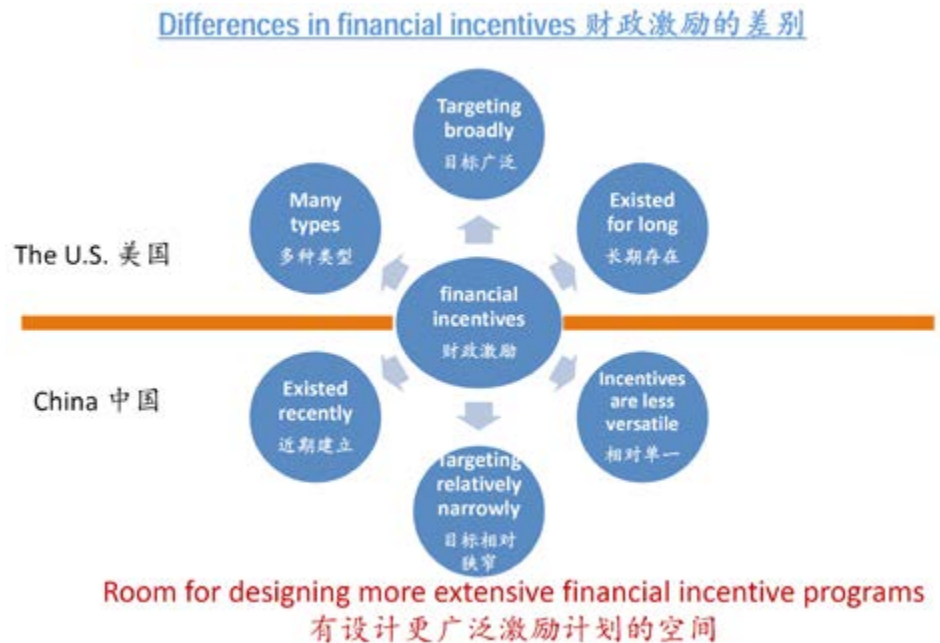


Figure 2. A comparison and recommendation result from policy studies on building energy efficiency, distributed renewable energy, and green buildings, presented in Sanya in July 2012.

# Appendix G: Clean Vehicles Consortium Project Fact Sheets

## Advanced Batteries and Energy Conversion

Degradation Mechanisms in Li-Ion Batteries†	
Characterization of Degradation Mechanisms in Li-Ion Batteries .....	G4
In-situ Neutron Depth Profiling of Lithium Ion Battery Materials for	
Improved Electrochemical Performance and Aging Models .....	G6
Li-ion Battery Aging and Internal Degradation Mechanisms .....	G8
Understanding the Performance and Reliability of Large Format Li-Ion Batteries	
through In-situ Time-resolved Neutron Diffraction 3D Mapping* .....	New Project*
New Battery Chemistries†	
High Energy Density Battery Chemistries .....	G10
Fundamental Understanding of Lithium Air Reaction Mechanisms .....	G12
Battery Implementation .....	
Modeling and Control of Lithium-Ion Batteries .....	G14

## Advanced Biofuels, Clean Combustion, and Auxiliary Power Unit (APU)

Fundamental Autoignition Chemistry of Advanced Biofuels.....	G16
Chemical and Physical Models for Novel Fuels .....	G18
In-Cylinder Biofuel Combustion Behavior .....	G20
Integrated Powertrain and Aftertreatment System Control for Clean Vehicles .....	G22
Development of APU-Oriented Boxer Engine .....	G23
APU-Oriented High Efficiency and Clean Combustion System .....	G25
Integration and Systematic Control of APU System.....	G27
Energy Conversion.....	G28

## Vehicle Electrification

Efficient and High Power Density Electric Powertrain .....	G29
Control and Optimization of Distributed Vehicle Network .....	G30
System Integration of Electrified Vehicles†	
Rapid System Integration through Modular Configuration, Sizing, and Control for Hybrid Vehicles.....	G31
Intelligent Fault Diagnosis and Prognosis.....	G33
Battery Modeling and Control†	
Adaptive Battery Management System On and Off the Grid.....	G35
Data-Based Techniques for Battery-Health Prediction .....	G37

## Advanced Lightweight Materials and Structures

Forming Processes for Lightweight Materials .....	G38
Cost Effective Lightweight Materials .....	G39
Joining in Multi-Material Vehicle Structures†	
Dynamic Characterization of Spot Welds for Advanced High Strength Steel .....	G40
High Density Battery Chemistries .....	G41
Hybrid Friction Stir Welding for Dissimilar Materials .....	G43
Hybrid Materials Interface Increased Strength Method and Modeling* .....	New Project*
Multi-Material Lightweight Body Subsystem and Vehicle Optimization.....	G44

## Vehicle-Grid Integration

Information Grid for Electrified Vehicles†	
System Architecture and Interaction Mechanism of ITS Based V2G .....	G46
EV Intelligent Control Based on Vehicle-Grid-Infrastructure Interaction .....	G48
Vehicle-Grid System Modeling for Technology Deployment.....	G49
Control Strategies for Vehicle-Grid Integration.....	G51
A Wireless Magnetic-Resonance Power Transmission System for EV Charging* .....	New Project*

## Energy Systems Analysis, Technology Roadmaps, and Policy

Set CV Technology Energy Efficiency and GHG Targets and Evaluate Life Cycle Performance .....	G53
Fuel Mix Strategies and Constraints .....	G55
Fuel Economy and GHG Standards and Labels for PEVs from a Life Cycle Perspective .....	G57
Fleet Modeling on China's In-use Vehicle Fleet .....	G59
Electricity and Material Sourcing Scenario Analyses to Guide Vehicle Technology Strategies.....	G60

† Indicates projects that have fact sheets provided at the subtask (major tasks within a project) level.

\* Indicates new projects for CERC CVC; fact sheets from year 2 are not available for these recently established projects.

## Research Topics

The Clean Vehicles Consortium (CVC) research is organized into six thrusts. An overview of progress and major activities is provided below, followed by additional details for projects within each thrust.

### *1. Advanced Batteries and Energy Conversion*

High cost and insufficient reliability are still the main limiting factors for the success of electrified vehicles. The effort on deeper understanding of battery degradation mechanisms produced new results. The coarsening of cathode nanoparticles was observed with atomic force microscope and scanning electron microscope micrographs, the effect of which on cathode performance was evaluated with X-ray micro tomography. During cell aging, the porosity increases and result in loss of contact between cathode nanoparticles and the carbon matrix. For  $\text{FePO}_4$  cells, porosity also affects the three-phase boundary between the nanoparticles, electrolyte, and carbon matrix, causing incomplete phase transformation. In parallel, we are also building a large-scale molecular dynamic simulation model to understand the degradation of batteries. Outcome from these models can help understand critical topics such as the irreversible reactions on lithium-air batteries, or design processes that better passivate cathode oxide surfaces and prevent manganese dissolution, which is known to be a major reason for capacity-fade in spinel oxide-based battery.

Over the past year, through industrial members' support, CERC CVC launched a second project focusing on the modeling and estimation of battery state of health, complementing an existing project supported by U.S. Department of Energy funds. Both projects focus on the lithium iron phosphate chemistry and use two different approaches to estimate battery degradation. The outcome of these studies will help identify capacity fade and anode solid-electrolyte-interface thin-film growth, which are critical factors to reflect battery energy and power capabilities.

### *2. Advanced Biofuels and Clean Combustion*

Despite of the fact the production of domestic crude oil and natural gas surged in the last couple of years, CERC CVC believes it is important to continue studying the combustion of biofuels and engine design for electrified vehicles. In the near term, engines can be much more efficient and smaller when they are part of a hybrid powertrain. These more-efficient engines need to be more accommodating to fuels produced from a wider array of renewable sources. A basic step to enable fuel-flexible engines is to obtain broad and detailed characterization of the chemistry and physics related to autoignition, which enables cleaner and more-efficient combustion. Both experimental and simulation methods are used to understand the kinetic mechanisms, which can then be used to predict the combustion behavior of various renewable fuels.

Engines that are part of the hybrid powertrain can operate in a narrower speed and power range, enabling innovation for better combustion efficiency; improved noise, vibration, and harshness performance; and deployment of simple/compact/lightweight designs that were not possible on traditional vehicles. The potential for innovation is particularly high for the small range-extender engine on a plug-in hybrid vehicle. These engines are called auxiliary power unit (APU) engines. CERC researchers have been studying various aspects of the APU engine design, using a boxer-type engine as an example platform.

### *3. Vehicle Electrification*

In addition to adding batteries, several other subsystems are needed to build a complete electrified powertrain: motors, power electronics, transmission, and controls. Projects in this thrust area aim to develop modeling, analysis, and simulation tools to enable fast and efficient designs of these subsystems. In recent years, there has been significant effort in the pursuit of high-energy-density and high-efficiency motors, especially those using less or no rare earth material. One limiting factor in the pursuit of high-power-density motors is overheating. Therefore, efficient simulation methods to accurately predict not only the electrical and magnetic behaviors, but also the thermal behavior are needed. Computationally efficient two- and three-dimensional steady-state solvers for synchronous and asynchronous machines have been developed over the last year.

About 90% of the hybrid electric vehicles sold in the U.S. market are power-split hybrid vehicles with a single planetary gear; three of the examples are the Toyota Prius, Ford Fusion, and Chevy Volt. A CERC project focuses on extending the power-split design concepts to heavy hybrid vehicle applications. Automated modeling and powertrain analysis tools make it possible to exhaustively search through all possible configurations in order to identify an efficient powertrain design and control algorithm, including optimal mode switching.

### *4. Advanced Lightweight Materials and Structures*

Lightweighting is an efficient and reliable way to reduce fuel consumption, regardless of the powertrain technology. The main focus of research projects in this thrust area is to develop high-quality and economical joining processes for lightweight materials, especially between dissimilar materials, especially for aluminum alloys and advanced high-strength steels. Methods to non-destructively estimate the joining quality, e.g., spot welding, are important to connect weld quality to predicted structure integrity during a crash. An optimization method for multi-material vehicle body subsystems incorporating criteria for manufacturability and ease of assembly was developed, as was a mini-ethylene-carbonate body structure to demonstrate the optimization methodology.

### *5. Vehicle Grid Integration*

Electrified vehicles promise to reduce the transportation sector's reliance on fossil fuels, but plug-in electric vehicles (PHEVs) or pure electric vehicles (EVs) may increase the grid load. In addition, the reduced range may change traffic patterns. Projects in this area aim to model and analyze the interaction of the vehicles, grid system, and intelligent transportations, and to learn how the intelligent transportation and smart grid systems can help to accommodate PHEVs and EVs. Possible questions to be answered include the placement of charging stations, decentralized charging strategies, and real-time strategy to locate recommended charging stations for vehicles needing charging. Models that capture these interactions have been developed and analysis and simulation results have provided insight into the best practices in the control and design of the future vehicle-grid system.

### *6. Energy Systems Analysis, Technology Roadmaps, and Policy*

The impact of any new process or technology must be evaluated in a comprehensive and holistic way. As an example, an electrification or lightweight technology result in carbon footprint reduction cannot be examined only through the use phase. Life cycle analysis of various technologies studied in the CERC CVC aim to provide that holistic view and form the basis of technology roadmaps and policies. The life cycle models developed in this thrust area encompass both the vehicle life cycle (materials production, manufacturing, operation, and end-of-life management) and the total fuel cycles (upstream and combustion). These models were developed to have functional equivalence (e.g., gradeability) and consider key physical limits (e.g., engine knock and flammability limit) so the comparison of baseline and "clean vehicle" cases is realistic. These concepts can form the basis of future fuel economy and greenhouse gas standards that reflect life cycle emissions rather than just use-phase emissions.



## Advanced Batteries and Energy Conversion

# Characterization of Degradation Mechanisms in Li-Ion Batteries

Joint Project

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>The Ohio State University</li> <li>Argonne National Laboratory</li> <li>University of Michigan</li> <li>Sandia National Laboratories</li> <li>Oak Ridge National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> <li>Beijing Institute of Technology</li> </ul>

## Research Objectives

The project team aims to improve the robustness of current-generation lithium-ion batteries via detailed characterization of degradation and aging mechanisms. In addition, the project is formulating design principles based on the knowledge of degradation and aging mechanisms to improve battery cycle life.

## Technical Approach

- Generate aged cells by accelerated electro-thermal protocols that are representative of actual driving conditions for electric vehicles (EVs), hybrid EVs (HEVs), and plug-in HEVs
- Conduct multi-scale *ex situ* analysis of the anodes and cathodes harvested from unaged and aged cells for changes in physical and morphological structures, surface deposits, micro structures, phase fraction, active lithium concentration, etc.
- Perform electrical and electrochemical characterization at nanoscale using an atomic force microscope (AFM)
- Apply the aging mechanism data to calibrate and evaluate the microscale models for battery performance

## Significant Results

The first step was for the project team to acquire, through industrial partnership, new prismatic cells used in EV production. The research team followed through on work completed in Fiscal Year (FY) 2011, when researchers used AFM and scanning electron microscopy micrographs to observe coarsening of cathode nanoparticles. In FY 2012, researchers used X-ray microtomography to evaluate the coarsening's effect on the composite cathode structure's porosity. These

experiments were conducted on materials harvested from spiral-wound cylindrical cells, previously subjected to aging tests of repeated conditions (C-rate, temperature, state of charge), until 20% capacity loss was achieved. The sample cells were then completely discharged and disassembled to harvest samples from the positive electrode.

The project made several findings, including that porosity measured on samples harvested from the core of the cylindrical cell was higher when compared to samples harvested from the periphery of the same cell. This is possible due to the electrode stacking stress and the peak temperatures at the core of the cylindrical cell. Comparing across cells aged with different protocols, the porosity was higher for cells aged at a higher C-rate, possibly due to the cells being aged at a higher C-rate, possibly due to the result of rapid cyclic volume changes at a higher C-rate that cause loss of contact between cathode nanoparticles and the carbon matrix during the cell aging process.

Researchers also performed X-ray diffraction, which shows higher  $\text{FePO}_4$  phase fraction in aged cells. Change in porosity affects the three-phase boundary between the nanoparticles, electrolyte, and carbon matrix, causing incomplete phase transformation (see Figure 1). Current sensing AFM maps of aged samples showed lower surface conductivity (see Figure 2).

The aged cathode surface is harder than the unaged ones. Such changes in nanomechanical properties cause degradation in battery performance.

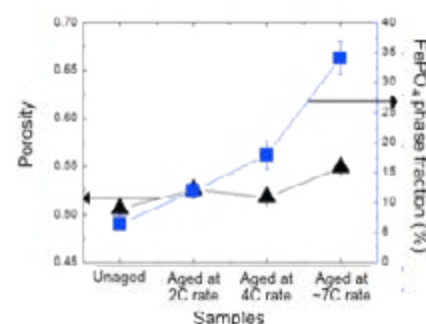


Figure 1. Change in porosity and phase fraction with aging. Figure 1. Change in porosity and phase fraction with aging.

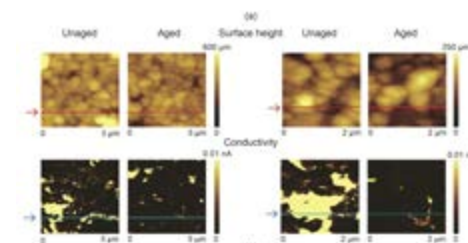


Figure 2. Surface height and conductivity variation with aging.

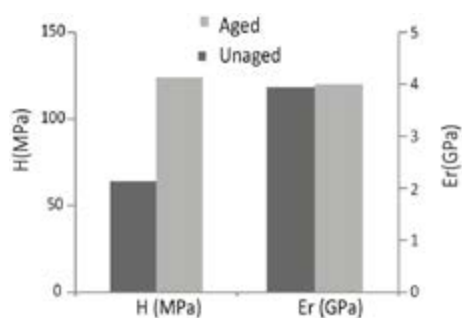


Figure 3. Hardness in unaged and aged samples.

### Future Plans

The team has recently acquired new lithium-ion prismatic cells from the industry partners for conducting a new campaign of aging characterization tests to continue the material degradation studies. The team will continue efforts to design aging protocols for the acquired prismatic cells. The team will study the effect of shape and cell design on these cells through the multi-scale characterization plan, as well as the percolation properties of unaged and aged cathodes. The team also plans to further advance the electron energy loss spectroscopy (EELS) methodology with the new Titan electron microscope for element identification and chemical structure. Finally, an *in situ* AFM electrochemical cell will be developed for morphological and diffusion studies of the electrodes.

### Expected Outcomes

- A refined EELS methodology for light element analysis in battery materials
- *In situ* AFM capabilities for direct analysis of morphological changes and electrochemical performance
- A robust understanding of aging mechanisms in batteries as a function of aging protocols and cell design and shape
- Parameters to quantify and relate evolution of microstructure in the cathode with the system-level aging metrics

## Advanced Batteries and Energy Conversion

# In-situ Neutron Depth Profiling of Lithium Ion Battery Materials for Improved Electrochemical Performance and Aging Models

Cooperative Project (U.S.)

## U.S. Research Team Lead

- Tsinghua University
- Beijing Institute of Technology

## U.S. Partners

- The Ohio State University

## Research Objective

The objective of this project is to establish a direct method to measure the concentration of active material in the anode and cathode of lithium-ion batteries through neutron depth profiling (NDP). The information obtained from *ex situ* and *in situ* NDP will be used to improve understanding of the lithium diffusion in electrodes during cycling operations, develop quantitative methods to measure lithium buildup in the interface region of the negative electrode (the solid electrolyte interface [SEI] layer), and improve results of electrochemical lithium-ion cell models for performance and aging prediction.

## Technical Approach

- Improve capabilities of *ex situ* and develop *in situ* methodology for the analysis of lithium-ion electrode materials at The Ohio State University's (OSU's) Research Reactor
- Develop a lithium-ion coin cell design, enabling for *in situ* NDP measurements
- Conduct *in situ* and *ex situ* NDP to quantify the lithium concentration in the surface region of electrodes and relate to cell-level testing results (electrochemical impedance spectroscopy, cycling data, calorimetry)
- Achieve a systematic design of an experiment to evaluate the lithium concentration profile in electrode samples harvested from new and aged cells and relate the experimental results to cell usage data
- Analyze experimental results from *in situ* and *ex situ* NDP of lithium-ion cell electrodes through electrochemical modeling that is inclusive of aging (e.g., SEI growth models)

## Significant Results

During the first year, the existing NDP facility at OSU was improved to enable one to conduct systematic *ex situ* and *in situ* studies. A two-gas system was built for safe loading/unloading of air sensitive battery samples and to create an inert gas environment during the NDP experiments. Specifically, argon gas was used in the pre-chamber built around the NDP chamber to enable loading/unloading of air-sensitive samples (Figure 1).

Helium gas was supplied to the NDP chamber with the option to control the chamber pressure from atmospheric conditions to vacuum (10-6 Torr) (Figure 2). This enables one to conduct *ex situ* NDP tests (typically done in vacuum) as well as test samples under helium gas at controlled pressure, which is necessary for *in situ* studies of lithium-ion cells operating with liquid electrolytes.

The developed testing facility was benchmarked against the result of *ex situ* NDP studies previously conducted at the National Institute of Standards and Technology (NIST) on electrode samples harvested from aged lithium-ion batteries. The lithium concentration profiles measured at the NIST facility and the modified OSU-NDP facility show excellent agreement in terms of shape, concentration, and depth values (Figure 3).

The developed testing facility was also used to evaluate the *in situ* capabilities by testing one of the samples in a helium environment at 1 standard atmosphere.

Conducting NDP under a helium gas environment as a possible *in situ* approach has not been reported in the literature and will be one of the key novelties of this project.



Figure 1. Overview of the OSU NDP instrument with modified chamber.

## Future Plan

The main contribution of this project includes the development of an *in situ* NDP technology and its applications to lithium-ion battery studies to improve the understanding of lithium transport within electrodes and interface processes that occur during cycling behavior of new and aged batteries.

This diagnostic tool complements the multi-scale characterization studies that are being conducted at OSU to investigate the degradation mechanisms in lithium-ion battery materials due to cycle aging.

The logical path for achieving *in situ* NDP includes the exploration of a "half-cell" design, a windowless concept with inert gas sample environment, and a study of lithium cells with low vapor pressure.

The unique ability of NDP to provide non-destructive and quantitative measures of lithium concentration in the surface region of electrodes will provide essential data for improved electrochemical performance and aging models. The aging models can then predict the life of

the battery with a higher confidence level and can prove vital in diagnostic and prognostic applications for full-scale, production-level batteries.

### Expected Outcomes

- Demonstration of the *in situ* NDP capability through an approach combining half-cell design and controlled NDP testing conditions
- Definition of methods to combine the *ex situ* and *in situ* NDP experimental results with the design and calibration of system-level electrochemical models for lithium-ion battery performance prediction
- Investigation of the growth of the SEI layer in lithium-ion cell anodes with NDP-based methods to provide dynamic information for modeling and simulation
- Collaborations created with Chinese and industrial partners to develop applications of NDP-based measurement techniques

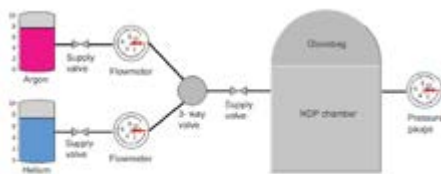


Figure 2. Schematic of the gas supply system for the NDP chamber.

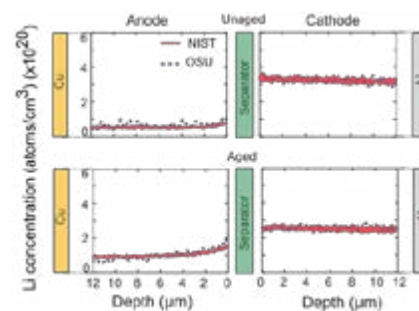


Figure 3. Comparison of lithium concentration profiles in unaged and aged lithium-ion battery electrodes.



## Advanced Batteries and Energy Conversion

# Li-ion Battery Aging and Internal Degradation Mechanisms

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
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## Research Objectives

The objective of this project is to predict atomic-length-scale cathode degradation mechanisms (e.g., Mn(II) dissolution) from spinel  $\text{LiMn}_2\text{O}_4$  oxides, a promising prototype material for cathodes in lithium-ion batteries. In addition, the project is investigating electrolyte decomposition on the oxide surface, possibly synergistic with  $\text{LiMn}_2\text{O}_4$  degradation. A second objective is to apply similar methods to study the stability of electrolytes on lithium-air cathode surfaces. This work is synergistic with Don Siegel's Clean Energy Research Center high-energy-density battery project.

## Technical Approach

- Implement electronic structure density functional theory (DFT), including DFT with Hubbard augmentation of d-electrons ("DFT+U") and hybrid DFT functionals
- Use both geometry optimization and finite-temperature molecular dynamics calculations

## Significant Results

The project team has proposed a new reconstruction of  $\text{LiMn}_2\text{O}_4$  (111) surface (Figure 1). This predicted reconstruction yields a surface energy lower than that of the (100) surface, consistent with the experimental finding that (111) facets are most prominent.<sup>1</sup> The project team's predicted (111) surface is slightly higher in energy (0.73 joules per square meter [ $\text{J}/\text{m}^2$ ]) than the surface predicted by the group at Lawrence Berkeley National Laboratory.<sup>2</sup> The latter involves manganese-lithium exchange in subsurface oxide layers (0.66  $\text{J}/\text{m}^2$ ).

The main reason for pursuing a new surface reconstruction is that, unlike Karim et al.'s (111) surface, the present surface exhibits exposed (5-coordinated) manganese ions. Because it is well known that Mn(II) dissolves from spinel  $\text{LiMn}_2\text{O}_4$  into the liquid electrolyte, manganese must become exposed after cycling power. This implies that manganese ions must migrate to the surface even if, in as-grown crystals, they are not thermodynamically the most favorable there. The project's (111) reconstruction is thus at least a potential intermediate configuration that exists just prior to manganese dissolution.

The two (111) surfaces exhibit dramatically different reactivity toward the organic-solvent-based electrolyte used in lithium-ion batteries. Here the focus is on the decomposition of ethylene carbonate (EC) molecules, a critical component of electrolytes, on the predicted surfaces. EC does not appear to react with Karim et al.'s reconstructed (111) surface, which is terminated with lithium and oxygen ions; all EC reactions examined so far are endothermic. However, EC molecules coordinated to exposed 5-coordinated manganese ions on the proposed (111) surface react exothermically to break two different carbon-oxygen bonds (Figure 2). This result dovetails with the project's findings on the less stable  $\text{LiMn}_2\text{O}_4$  (100) surface.<sup>3</sup> It further suggests the following larger perspectives:

- EC coordination to exposed manganese may be required for reactions
- If manganese that is exposed on the oxide surface indeed always leads to EC decomposition, such decomposition and manganese dissolution must be strongly correlated. If the premise is true, these events cannot occur independently

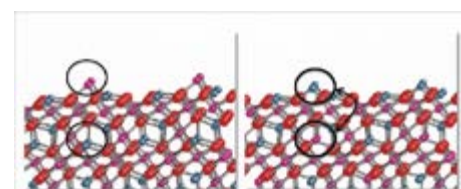


Figure 1: Karim et al.'s reconstruction involves exchange of surface lithium and subsurface manganese ions. The project team's proposed reconstruction involves simply the removal of  $\text{LiMn}_2\text{O}_4$  formula units on the surface (not shown). Red, pink, and grey spheres are oxygen, lithium, and manganese ions, respectively.

## Future Plans

The immediate future plan is to calculate the reaction barriers, as well as later steps of EC decomposition, which can include loss of proton; EC oxidation; and ultimately, removal of manganese from the oxide surface. In outlying years, the effect of defects and nickel substitution on spinel oxide surfaces will be examined.

- 1 M.R. Huang, C. W. Lin, H. Y. Lu, "Crystallographic faceting in solid-state reacted  $\text{LiMn}_2\text{O}_4$  spinel powder," *Appl. Surf. Sci.* 177, 103 (2001).
- 2 A. Karim, S. Fosse, and K. Persson, "Surface structure and equilibrium particle shape of the  $\text{LiMn}_2\text{O}_4$  spinel from first-principles calculations," *Phys. Rev. B* 87, 075322 (2013).
- 3 K. Leung, "First-Principles modeling of the Initial Stages of Organic Solvent Decomposition on  $\text{LiMn}_2\text{O}_4$  (100) Surfaces," *J. Phys. Chem. C* 116, 9852 (2012).

### Expected Outcomes

- Understanding of the detailed, atomistic mechanisms of manganese dissolution from spinel  $\text{LiMn}_2\text{O}_4$  surfaces and electrolyte decomposition is expected to yield insight that can better passivate such cathode oxide surfaces and prevent manganese dissolution, which is known to be a major reason for capacity fade in spinel oxide-based batteries
- Ability to inform rational design of electrolyte additives or inorganic coatings that can prevent such degradation
- Related insights that are particularly pertinent for nickel-doped high-voltage cathode materials that can more readily oxidize the electrolyte and cause further capacity fade in batteries

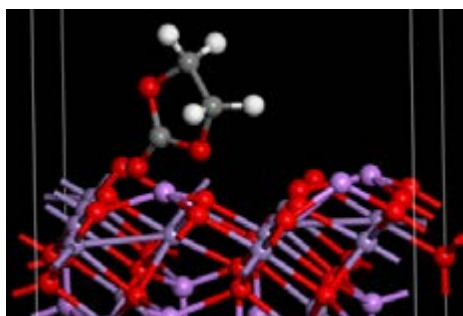


Figure 2a. Physisorbed EC,  $\Delta E = 0.00$  electron volts (eV).

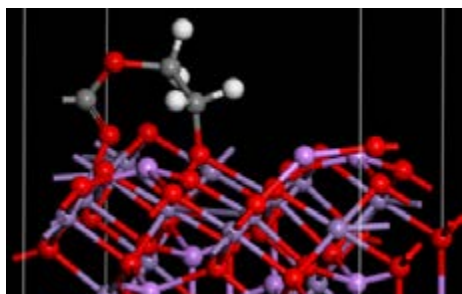


Figure 2b. Chemisorbed EC,  $\Delta E = -0.49$  eV.

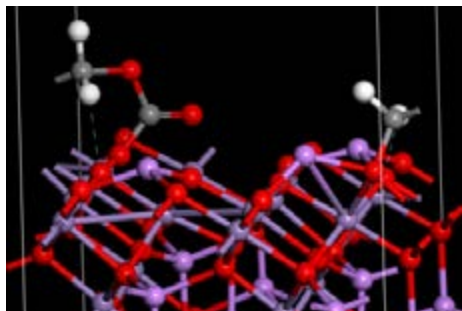


Figure 2c. Another chemisorbed EC,  $\Delta E = -0.20$  eV.

## Advanced Batteries and Energy Conversion

## High Energy Density Battery Chemistries

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
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*Research Objective*

This project is increasing understanding and developing practical guidance for the design of next-generation batteries that promise substantial increases in energy density and/or safety. This includes lithium-sulfur and lithium-air batteries, the use of solid electrolytes in lithium-ion batteries, and batteries that shuttle ions other than lithium.

The recent discovery of solid electrolytes that boast lithium conductivities on par with those of liquid electrolytes has opened the door to the application of solid electrolytes in commercial batteries. Solid electrolytes offer many advantages over liquid electrolytes—most notably, increased safety. Solid electrolytes also promise to improve the cycle life of lithium-sulfur batteries because solid electrolytes prevent the dissolution of sulfur, which plagues lithium-sulfur batteries that use liquid electrolytes.

There is also a need to explore battery concepts that go beyond lithium. For example, identifying the primary mechanisms limiting the performance of rechargeable metal-air batteries (e.g., high charging potentials, poor reversibility, and limited capacity/capacity fade) will enable the development of rational strategies for improving battery performance. Such improvements can ultimately transfer from the laboratory bench to commercial application in electric vehicles. Other electrode chemistries for batteries that shuttle cations or anions suggest new opportunities.

Specific objectives of this project include the following:

- Determine the crystallographic and chemical properties of solid electrolytes that are responsible for high ionic conductivities and that lead to thermodynamic stability in high-voltage batteries
- Explore the viability of new classes of “beyond lithium-ion” battery concepts by combining of first-principles computational modeling of lithium-air battery materials

with parallel materials characterization experiments (at partner institutions)

- Elucidate key morphological features of  $\text{Li}_2\text{O}_2$  discharge phases in lithium-air batteries
- Calculate rates of charge and mass transport in  $\text{Li}_2\text{O}_2$  discharge phases and explore mechanisms for enhancing transport
- Uncover phenomena resulting in high charging potentials, poor reversibility, and limited capacity/capacity fade in lithium-air batteries

*Technical Approach*

- Predict electronic structure, thermodynamic phase stability, and a variety of important kinetic properties of electrode materials and solid electrolytes through the use of quantum mechanical and statistical mechanical computational techniques
- Combine the results of these first-principles calculations with coarse-grained continuum descriptions of the dynamic evolution of electrode and electrolyte materials at the macroscopic scale

*Significant Results*

**Solid electrolytes:** Undesirable reactions with the anode-liquid electrolyte interface plague the current generation of lithium-ion batteries. Replacing the liquid electrolyte with a solid electrolyte would solve many of these problems. The project team focused on two promising classes of solid electrolytes: a variety of phases in the lithium-phosphorus-sulfur (Li-P-S) system and its quaternary derivatives, and a new class of recently discovered anti-perovskite phases.

For the solid electrolyte phases in the Li-P-S system, researchers used combinatorial first-principles methods to identify the stable ordered arrangements of the highly mobile lithium ions over interstitial sites of phosphorus sulfide host crystal structures. This structural information is key to determining the factors that lead to high lithium mobility in these phases. Building on this insight, researchers

determined lithium-ion transport mechanisms in important compounds in the Li-P-S system.

The research team also identified phase stability and fast lithium transport mechanisms in a new class of anti-perovskite compounds having stoichiometry  $\text{Li}_3\text{OX}$  with X = chlorine, bromine. These insights will provide guidance in the design and discovery of other promising solid electrolyte phases.

**Na-ion batteries:** A Tsinghua University research student examined differences between electrodes for sodium (Na) batteries and similar electrodes for lithium batteries. Particular focus was placed on the  $\text{Na}_x\text{TiS}_2$  system, to elucidate phase transformations that occur during various points of charge. While sodium diffusion mechanisms are predicted to be comparable to those in the  $\text{Li}_x\text{TiS}_2$  counterpart, the sodium intercalation compounds are predicted to undergo a variety of structural changes during charge and discharge, which can be detrimental to battery lifetimes.

**New battery chemistries:** The project team also explored completely new battery concepts, including an oxygen-shuttling battery that operates at high temperatures similar to a fuel cell, with three times the electromotive force (EMF) of a solid oxide fuel cell.

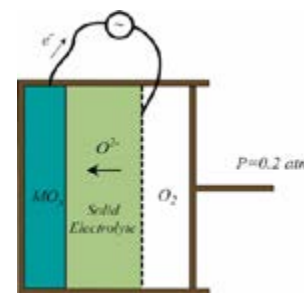


Figure 1. Oxygen-shuttling battery schematic with an oxygen (eventually air) cathode and titanium (Ti) or zirconium (Zr) anode that would form different oxides upon charging.

The new battery relies on an anode of pure titanium or zirconium; both can dissolve oxygen up to concentrations of 33% without significant structural change. If oxygen intercalates further to form TiO or ZrO, capacities as high as 960 milliamper-hours per gram (mAh/g) and 540 mAh/g, respectively, can be reached.

Researchers performed a first-principles study of relevant electronic, thermodynamic, and kinetic properties of both systems, determining that oxygen can easily intercalate into the crystal structures of titanium and zirconium with negligible volume change. In contrast to the formation of other metal oxides, these suboxide phases remain electronically conducting.

Using kinetic Monte Carlo, the project team predicted oxygen diffusion coefficients at solid oxide fuel cell operating temperatures that are similar to lithium-ion diffusion coefficients in lithium-ion batteries.

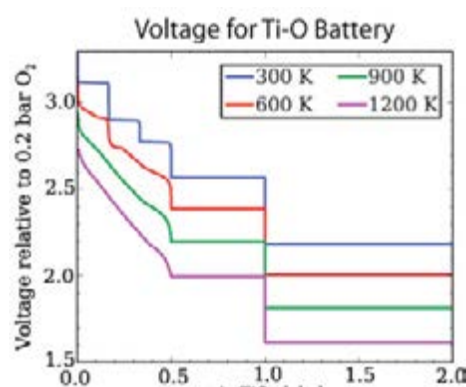


Figure 2. Predicted voltage curve for a titanium-air battery.

**Li-air batteries:** Rechargeable non-aqueous lithium-air batteries are increasingly attracting attention as a potentially transformative energy storage technology due to their high theoretical specific energy density. In the absence of undesirable side reactions (e.g., degradation of the solvent or carbon support), a lithium-air cell can be described by the reversible reaction  $2\text{Li} + \text{O}_2 \leftrightarrow \text{Li}_2\text{O}_2$ . This chemistry is unlike conventional lithium-ion intercalation electrodes: the solid-phase discharge product, lithium peroxide ( $\text{Li}_2\text{O}_2$ ), nucleates and grows on the cathode during discharge and subsequently decomposes during recharge.

In order to achieve a high energy density, the cathode of a lithium-air cell should be substantially filled with  $\text{Li}_2\text{O}_2$  at the end of discharge. However, prior studies have suggested that charge transport limitations through an ostensibly insulating  $\text{Li}_2\text{O}_2$ -air system is the mechanism and efficiency of charge transport through the discharge product. Unfortunately, an accepted mechanism for charge transport in lithium-air cathodes has yet to emerge.

As a step toward elucidating the impact and mechanism of charge transport in lithium-air cells, the project's recent work employed first-

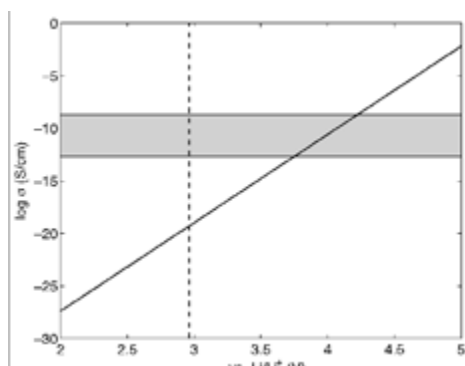


Figure 3. Predicted electronic conductivity as a function of cell voltage. The dashed line is the open circuit voltage, and the shaded region indicates the target conductivity.

principles calculations to predict conductivity at surfaces and in the bulk of  $\text{Li}_2\text{O}_2$ . Regarding bulk transport, the project team predicted the concentrations of all chemically relevant intrinsic (point) defects in  $\text{Li}_2\text{O}_2$ , as well as the mobilities of the dominant charged species, as a function of cell voltage.

Figure 3 summarizes the project team's findings with respect to conduction in bulk  $\text{Li}_2\text{O}_2$ . Negative lithium vacancies and small hole polarons are identified as the dominant charge carriers. The electronic conductivity associated with polaron hopping ( $5 \times 10^{-20}$  S/cm) is comparable to the ionic conductivity arising from the migration of lithium ions ( $4 \times 10^{-19}$  S/cm), suggesting that charge transport in  $\text{Li}_2\text{O}_2$  occurs through a mixture of ionic and polaronic contributions. These data indicate that the bulk regions of crystalline  $\text{Li}_2\text{O}_2$  deposits are insulating, with appreciable charge transport occurring only at high charging potentials that result in partial delithiation.

Achieving high discharge capacities will depend upon the presence of alternative charge transport mechanisms that bypass bulk transport. Figure 4 summarizes some of these mechanisms. Panel (a) corresponds to tunneling

through thin  $\text{Li}_2\text{O}_2$  films, which results in low capacity; panel (b) shows transport through bulk (which is insulating and therefore unlikely; and panels (c) through (e) illustrate possible higher-conductivity alternative pathways.

### Future Plans

The project will extend fundamental studies of the factors that produce stable and fast ion-conducting solid electrolytes by focusing on additional classes of solid electrolyte chemistries and crystal structure. These studies will broaden and strengthen design principles with which to discover superior solid electrolytes for lithium-ion batteries and for lithium-sulfur batteries. At the same time, researchers will continue exploring other battery concepts from first principles, including the following:

- Identify the most promising dopants/ electrolyte additives to enhance conductivity in  $\text{Li}_2\text{O}_2$
- Characterize the properties and performance of other non-lithium-based metal-air chemistries
- Expected Outcomes
- Design principles for rapid discovery of new solid electrolytes for the next generation of high-energy density batteries
- New battery concepts that go beyond lithium-ion
- Joint publications involving Anton Van der Ven's group at University of Michigan and Xiangmin He's group at Tsinghua University
- Identification of mechanisms that most strongly impact the performance (rate capability, capacity, efficiency) of metal-air batteries
- Prediction of transport rates for lithium-ions and electrons/holes in  $\text{Li}_2\text{O}_2$  discharge phase
- Prediction of optimal dopants to improve conductivity of  $\text{Li}_2\text{O}_2$ —invention disclosure filed

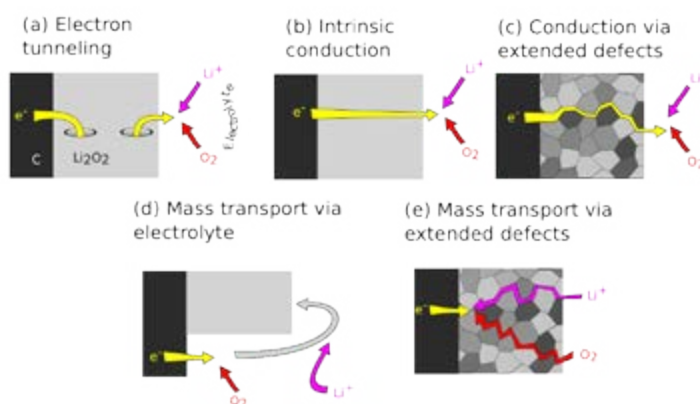


Figure 4. Hypothetical discharge mechanisms in a lithium-air cell, illustrating possible mass/charge transport pathways.



## Advanced Batteries and Energy Conversion

# Fundamental Understanding of Lithium Air Reaction Mechanisms

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
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## Research Objective

The objective of this project is to fundamentally understand reaction mechanisms in lithium-oxygen batteries. By combining electrochemical techniques with spectroscopic and imaging tools, researchers aim to gain new insights into the relationship between the surface chemistry and morphology of lithium-oxygen reaction products and device-level performance limitations such as low round-trip efficiency and short cycle life.

## Technical Approach

- Study the chemical stability of different cell components against lithium-oxygen reaction intermediates
- Characterize surface and bulk chemical composition of reaction products using spectroscopic techniques such as electron paramagnetic resonance (EPR) and X-ray absorption near-edge spectroscopy (XANES) in surface-sensitive total electron yield and bulk-sensitive fluorescence yield modes
- Study morphology and crystallinity of lithium-oxygen reaction products using transmission electron microscopy and scanning electron microscope imaging techniques

## Significant Results

**Chemical composition and charging kinetics of discharge products:** The team used XANES to study the relationship between surface and bulk chemistry and charging kinetics of  $\text{Li}_2\text{O}_2$ , which is the main discharge product in non-aqueous lithium-oxygen batteries. The results were published in the *Journal of Physical Chemistry Letters*.

This work has resulted in two major findings:

- The surface electronic structure of electrochemically formed  $\text{Li}_2\text{O}_2$  was different from the corresponding bulk structure

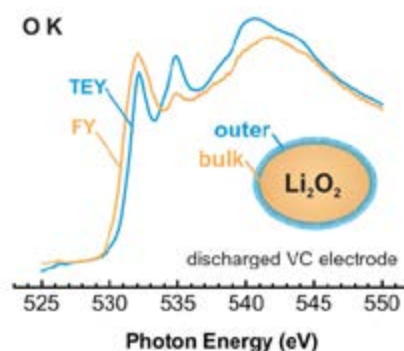


Figure 1. XANES characterization of the surface and bulk electronic structure of a discharged Vulcan carbon electrode.

- The voltage profile upon charging of  $\text{Li}_2\text{O}_2$  showed two regimes: a sloped region at low overpotential representing a solid solution-like charging mechanism, followed by a flat region at higher overpotential showing two-phase bulk decomposition

Considering the different electronic structures of surface and bulk  $\text{Li}_2\text{O}_2$  observed, the researchers hypothesize that the first regime corresponds to delithiation of surface  $\text{Li}_2\text{O}_2$ , which is followed by oxidation of bulk  $\text{Li}_2\text{O}_2$  in the second regime. This study therefore correlates observed charging kinetics to variations in surface electronic structure. Findings could yield insights for the design of practical lithium-air batteries with high round-trip efficiency.

**Lithium-oxygen reaction intermediates:** The team is using the rotating ring disk electrode technique to detect soluble intermediates of the lithium-oxygen reaction. The rotating ring disk assembly consists of a working electrode

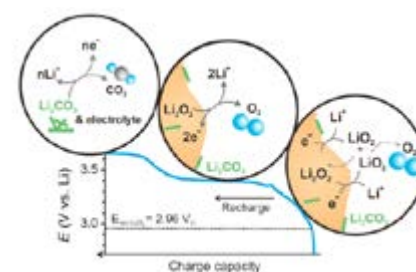


Figure 2. Proposed charging process of  $\text{Li}_2\text{O}_2$ .

surrounded by an annular gold ring, both of which can be independently polarized. By rotating the assembly, soluble species generated at the disk during the oxygen reduction reaction (ORR) and oxygen evolution reaction will be convected to the ring to be oxidized or reduced.

Cyclic voltammograms were obtained by sweeping the disk between 2.0 and 4.5 volts (V) versus  $\text{Li}/\text{Li}^+$ , while the ring was held at 3.5 V versus  $\text{Li}/\text{Li}^+$ , to oxidize any mobile reaction intermediates under both static and rotating

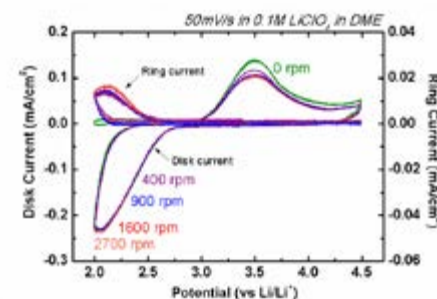


Figure 3. Cyclic voltammograms obtained at 50 millivolts per second (mV/s) in  $\text{O}_2$ -saturated 0.1 molar (M)  $\text{LiClO}_4$  in dimethoxyethane (DME) from 0 to 2,700 revolutions per minute (rpm).

conditions. When rotating the assembly at 400 revolutions per minute and above, there is an increase in the ring current, indicating the oxidation of a soluble ORR intermediate. This finding is in agreement with the hypothesis that the ORR mechanism proceeds via an intermediate step to produce  $\text{LiO}_2$  ( $\text{Li}^+ + \text{O}_2 + \text{e}^- \rightarrow \text{LiO}_2$ ), followed by the generation of  $\text{Li}_2\text{O}_2$  either by disproportionation ( $\text{Li}_2\text{O}_2 \rightarrow \text{Li}_2\text{O}_2 + \text{O}_2$ ) or concerted electron transfer ( $\text{Li}^+ + \text{e}^- + \text{LiO}_2 \rightarrow \text{Li}_2\text{O}_2$ ). The team is extending this method to study formation kinetics and reactivity of the  $\text{LiO}_2$  species at different potentials in different electrolyte solvents such as DME and dimethyl sulfoxide.

### Future Plans

Future experiments will include *in situ* EPR experiments to directly investigate reactivity of lithium-oxygen reaction intermediates. The project will also conduct scanning transmission X-ray microscopy for nanoscale chemical imaging and visualizing spatial distribution of  $\text{Li}_2\text{O}_2$  and  $\text{Li}_2\text{O}_2$  deposits in carbon-based and carbon-free lithium-oxygen battery cathodes.

### Expected Outcomes

- Determination of factors affecting  $\text{LiO}_2$  reactivity with electrodes and electrolyte solvents
- Optimized cathode materials for lithium-oxygen batteries with high activity toward oxygen reduction and evolution but minimal side reactivity with electrode/electrolyte components
- Design principles for the development of nanostructured lithium-oxygen battery cathodes with high geometric power capabilities as well as high gravimetric and volumetric energy densities

## Advanced Batteries and Energy Conversion

## Modeling &amp; Control of Li-Ion Batteries

Cooperative Project

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<ul style="list-style-type: none"> <li>Argonne National Laboratory</li> <li>University of Michigan</li> <li>Massachusetts Institute of Technology</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> <li>Beijing Institute of Technology</li> </ul>

*Research Objective*

This project will determine the factors that most strongly impact the performance of primary and secondary batteries. It will provide a theoretical basis for battery pack integration (battery series-parallel connection, battery size, battery radiation, etc.) and battery management (thermalelectrical safety) through multi-scale and multifaceted modeling. Researchers will work to understand performance variation of the battery pack and provide a theoretical basis for the battery matching and cell-to-cell balancing through experiments, modeling, and simulation. This project will also work to establish the SOC, SOH, and SOF algorithms as well as reduce capacity variation and extend battery life by balancing.

*Technical Approach*

- The phenomena of cell variations were examined through laboratory bench and vehicle demonstration. A battery pack model was established with sub-models of cell capacity fade, internal resistance, self-discharge, coulombic efficiency and thermal model. Simulation study on battery pack performances was carried out with different scenes of cell variations.
- An equivalent circuit model (ECM) with a consideration of contact resistance was established and further simplified to the Thevenin ECM. The model was implemented using vehicle demonstration data of 96 cells. Pseudo Ohmic internal resistances of 96 cells (POIRs) which are the sum of cell Ohmic internal resistances (COIRs) and contact resistances (CRs) were evaluated and further compensated by temperature influence. Shannon entropy is used to distinguish between the fault of the contact resistance and cell Ohmic internal resistance.
- Based on Matlab, through simulation studies, parallel-series and series-parallel configurations for battery packs were analyzed.

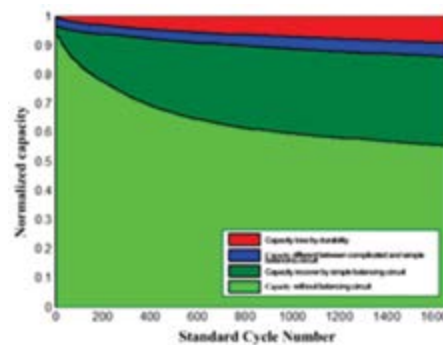


Figure 1: Pack capacity recovered by balancing.

*Significant Results*

The main results of this project include the following 3 aspects:

- Simulation study of battery cell variations
  - The sensitivity analysis of cell parameter variations was studied, and the main conclusions are listed as follows:
    - Coulombic efficiency, temperature, self-discharge rate are the main parameter which dominate the cell variations.
    - The design of thermal management should make sure the temperature difference is less than 5°C.
    - The dissipative equalization is sufficient for on-line equalization in EVs. The non-dissipative equalization is not essential for on-line equalization in EVs but is applicable for maintenance.
- Fault diagnosis based on cell variations
  - The faults of the battery pack such as loose connections, micro short circuit can be diagnosed by the inconsistency analysis of voltage, current, temperature, resistance, SOC and other parameters

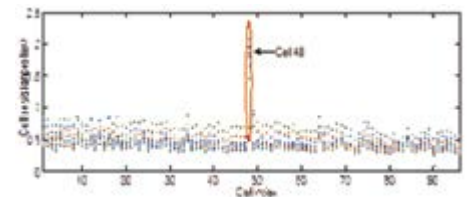


Figure 2: Variation of cell Ohm resistance.

- Shannon entropy can be used to differentiate between the fault of the contact resistance and cell Ohmic internal resistance.

## 3) Study of battery pack configuration

The advantages and disadvantages are discussed:

- Parallel-series configuration: BMS can measure the voltage of the parallel cells and thus needs fewer voltage measurement sensors results in low cost. Parallel cells have a good self-balancing feature. The reliability of the battery pack is relatively high with low cell reliability
- Series-parallel configuration: BMS can detect all cell states for precise management. The battery pack has higher safety when short-circuit or open-circuit happen in the cells. The BMS can accurately detect the failures in time.
- For battery pack construction, the pack configuration and pack parameters should be appropriately selected according to the requirement of the vehicle and cell parameters. BMS and corresponding management algorithms should match the pack configuration in order to optimal utilization of battery. Hybrid connections of the battery pack could be a better choice, it can prevent cells in parallel from releasing energy concentrated in a failed cell while the cells in parallel still has a self-balancing feature.

### *Future Plan*

- An accurate estimation of the battery pack capacity is significant for forecasting the EV driving range. But due to the diversiform driving conditions and the cell variations, it is difficult to accurately determine battery pack capacities in EVs by model prediction or direct measurement. At the same time, cell equalization strategies require cell capacity and SOC estimation in the battery. Thus precise battery pack capacity estimation is focused for the future plan.
- The cycle life is one of the most important characteristic of the battery. The cycle life of several commercial batteries, which are potential candidates of EV application, should be compared and studied.
- The driving range of electric vehicle is not easy to be precisely estimated, and the inaccuracy leads to range anxiety of EV passengers. One key problem is the prediction of battery remaining energy state. The effects of the battery energy state on the driving range and the estimation method of battery energy state are to be studied.

### *Expected Outcomes*

- Cycle life test and compare the battery cycle life
- Modeling of the battery capacity fade
- Investigate the aging mechanism
- Precise battery pack capacity estimation for EV driving range forecasting
- Cell capacity and SOC estimation for equalization strategies
- Determining the relationship of battery energy state and EV driving range estimation
- Estimation the battery energy state based on an electro-thermal battery model
- Optimize the battery energy prediction results based on newly-collected battery operating data



## Advanced Biofuels and Clean Combustion

# Fundamental Autoignition Chemistry of Advanced Biofuels

Cooperative Project (U.S.)

## U.S. Research Team Lead

- Craig A. Taatjes, Sandia National Laboratories
- Blake A. Simmons, Joint BioEnergy Institute,
- Sandia National Laboratories

- Angela Violi, University of Michigan
- Brandon Rotavera, Sandia National Laboratories
- Mohamad Akbar Ali, University of Michigan

## U.S. Partners

- Sandia National Laboratories
- Joint BioEnergy Institute
- University of Michigan

## Research Objective

Broad and detailed characterization of the chemistry and physics related to autoignition is of particular importance to national goals of renewable fuel use, such as those described in the Renewable Fuel Standard. The *Fundamental Autoignition Chemistry of Advanced Biofuels* focus area of the U.S.–China Clean Energy Research Center (CERC) effort considers a component-centered approach toward elucidating combustion fundamentals vital to the understanding of autoignition for application to fuel-flexible engines. Fuel ignition at lower temperatures is governed strongly by a sequence of reactions initiated by fuel radicals (R) reacting with molecular oxygen:  $R + O_2 \rightleftharpoons RO_2$ . The alkylperoxy radical  $RO_2$  adduct can undergo isomerization to a hydroperoxyalkyl radical, QOOH, the class of molecules responsible for ignition-controlling chain branching at low temperatures ( $< \sim 900$  Kelvin [K]). Understanding the molecular structure dependence of  $R + O_2$  chemistry is key for predicting performance of novel fuels and is a central focus of this part of the CERC effort.

In the past year, research has concentrated on a sesquiterpenoid fuel, bisabolane, that can be efficiently produced by engineered microbial fermentation of sugars liberated from lignocellulosic biomass. To approach the structurally complex target fuel, the research team selected two simpler fuels to represent the characteristic structural features (Figure 1).

## Technical Approach

- Use combined experimental and theoretical methods to determine fundamental reaction mechanisms for biofuel oxidation, especially autoignition processes that are critical for fuel-flexible, next-generation engines

## Experimental:

- Part I – Analyze high-resolution speciation of products from the first steps of laser-initiated oxidation of a branched alkane, 2,5-dimethylhexane (25DMH), and a cycloalkane, methylcyclohexane (MCH); examine approximately 25 reaction classes for these two prototype molecules to constrain the definition of reaction mechanisms of the observed products
- Part II – Take measurements of time-dependent OH and  $HO_2$  radical concentrations from pulsed laser-initiated oxidation of the three fuels

## Theoretical: Conduct *ab initio* simulations to identify reaction pathways

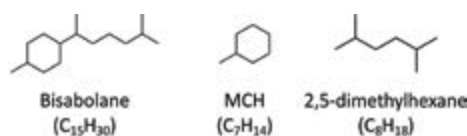


Figure 1. Oxidation chemistry of complex biofuels (e.g., bisabolane), studied both experimentally and computationally using structurally similar components.

## Significant Results

The two important classes of bimolecular product channels following  $O_2$ -addition to alkyl radicals (R) are OH- and  $HO_2$ -elimination. As the  $HO_2$  radical is relatively unreactive, its formation is associated with chain termination, but the OH radical is a highly effective chain carrier and is a marker for the QOOH radical chemistry that drives low-temperature chain branching and autoignition. To probe these channels for the test fuels, the project team conducted a multiplexed mass spectrometry experiment utilizing photoionization of molecular beams. These experiments can quantify the isomeric

coproducts of  $HO_2$  and OH in the  $R + O_2$  system and hence give detailed constraints on modeling of these reactions.

The oxidation of the test fuels was studied at two temperatures: 550 K and 650 K. Photolytically produced chlorine atoms abstract a hydrogen atom from the fuel molecule to form the initial radical R, which then reacts with  $O_2$ . Branching ratios for the coproduct of subsequent  $HO_2$  elimination (appearing at a mass 2 units smaller than the parent fuel) and the coproduct of OH elimination (appearing at the parent mass + 14) were quantified from their isomer-specific photoionization spectra.

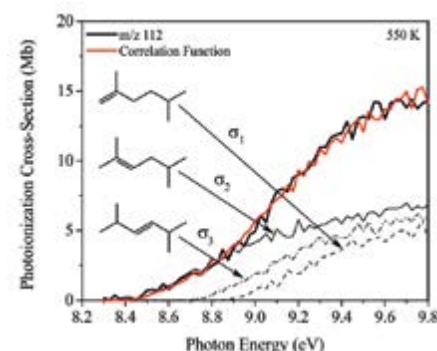


Figure 2. Photoionization spectra of the three coproducts of  $HO_2$ -elimination from 2,5-dimethylhexane. The fit to the pure component calibration spectra determines relative isomeric yields.

Reaction pathways leading to OH-elimination forming cyclic ether are of direct importance to low-temperature chain branching and promotion of autoignition. In measurements of 25DMH oxidation, the channel yielding 2,2,5,5-tetramethyltetrahydrofuran is predicted to be the dominant pathway toward formation of OH (Figure 3). Similar analyses were performed for MCH, the species representing the cyclic portion of bisabolane.

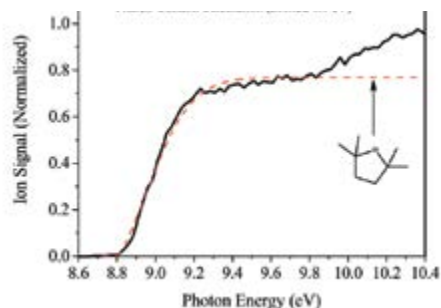


Figure 3. Photoionization spectrum of mass-to-charge ratio 128, representative of OH-elimination, compared to a theoretical calculation of the Franck-Condon spectrum of 2,2,5,5-tetramethyltetrahydrofuran.

### Future Plans

Ongoing analysis of experimental results and theoretical calculations are focused on the following specific areas:

- Short-term: OH/HO<sub>2</sub> concentration time histories for all three fuels indicated in Figure 1
- Long-term: Connection of component results to elucidate potential commonalities existing between the structurally complex biofuel (i.e., bisabolane) and the two analogs previously discussed

### Expected Outcomes

- Identification of the feasibility of constraining reaction pathways
- Rate coefficient calculations
- Connection of fundamental results to CERC focus areas involving engine tests

## Advanced Biofuels and Clean Combustion

## Chemical and Physical Models for Novel Fuels

Cooperative Project (U.S.)

## U.S. Research Team Lead

- Angela Violi, University of Michigan

## U.S. Partners

- University of Michigan

## Research Objective

The aim of this project is to develop kinetic mechanisms to predict the combustion behavior of various renewable fuels that can be used to replace current fossil fuels. Using a series of atomistic simulations, the project team is investigating the major reaction pathways of new bio-derived fuels, such as farnesane and bisabolane.<sup>1</sup> A detailed analysis is carried out to relate fuel formulation with combustion by-products and efficiency of combustion.

## Technical Approach

- Investigate systems of interest: methyl butanoate (MB), n-butylcyclohexane (n-BCH), and 2,6-dimethylheptane
- Employ density functional theory to perform *ab initio* simulations of reactants, intermediates, and products present in various reaction pathways
- Utilize Rice-Ramsperger-Kassel Marcus/master equation simulation solvers such as Multiwell to compute pressure- and temperature-dependent rate constants
- Assemble the kinetic mechanisms and validate them with experimental data
- Identify discrepancies between the kinetic model and experiments

## Significant Results

The main results of this project include developing the kinetic mechanisms, rate constants, and kinetic modeling of MB, n-BCH, and 2,6-dimethylheptane.

**Methyl-esters:** Figure 1 shows the new reaction pathways identified for the decomposition of MB.

In the high-temperature regimes, MB can decompose either through C-C and C-O bond fissions or through hydrogen migration reactions with bond breaking and forming, simultaneously. Pathways 1–5 depict homolytic C-C and C-O bonds fissions (barrierless), leading to the formation of two radicals. Pathways 6–10 (non-barrierless) are five hydrogen transfer reaction pathways. For all the pathways depicted in Figure 1, the rate constants were computed. Figure 2 provides an example, showing the comparison of the

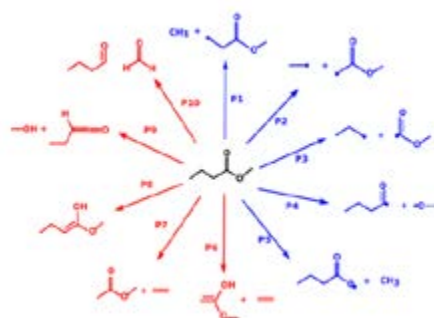


Figure 1. Ten new pathways for the unimolecular decomposition of methyl butanoate.

values obtained for Pathway 2 versus the data presented in the literature.

This study also highlights, for the first time, the importance of entropic contributions during unimolecular decomposition of MB. The rate

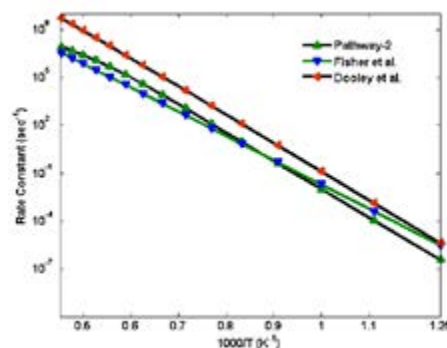


Figure 2. Comparison between the newly computed rate constants for Pathway 2 and data by Fisher et al.<sup>2</sup> and Dooley et al.<sup>3</sup>.

constants and branching ratio under different temperature ranges indicate that the main reaction pathway for thermal decomposition of MB is  $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(=\text{O})\text{OCH}_3 \rightarrow \text{C}_2\text{H}_5 + \text{CH}_2\text{C}(=\text{O})\text{OCH}_3$ , with less contribution from hydrogen migration channels.

**Cyclohexane (model compound of bisabolane):** Figure 3 illustrates the seven different unimolecular decomposition pathways of n-BCH that were analyzed.

At both temperatures, the updated model significantly improves the prediction of OH production; however, a discrepancy between the updated model and the experiment suggests further improvements are necessary.

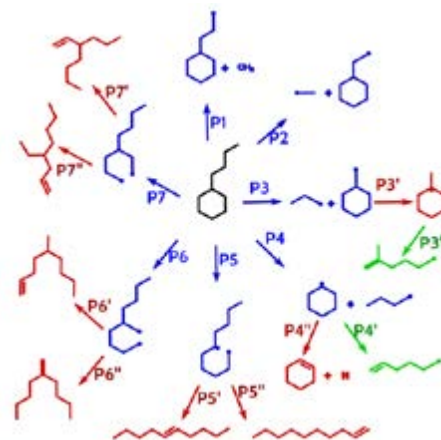


Figure 3. New decomposition pathways of n-BCH.

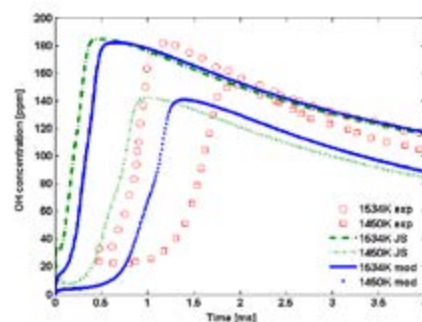


Figure 4. OH concentration profiles with new reaction pathways versus the original mechanism.

## Low-temperature oxidation of 2,6-dimethylheptane:

Dimethylheptyl radical (model compound of Farnesane), which leads to two major products; namely, alkene +  $\text{HO}_2$  and cyclic ether + OH, as shown in Figure 5.

The focus is computation of potential energy surfaces of 2,6-dimethylheptyl radical + O<sub>2</sub> reaction. Using the results, the project team implements *ab initio* transition state theory based on the master equation calculation to determine pressure- and temperature-dependent rate constants.

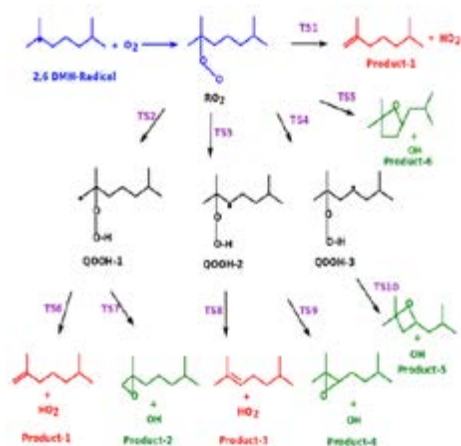


Figure 5. Reaction pathways for the oxidation of dimethylheptyl radical.

### Future Plans

The researchers will investigate the combustion behavior of new biodiesel molecules, such as farnesane and bisabolane.

### Expected Outcomes

- Low-temperature chemistry of farnesane and bisabolane
- Rate coefficient calculations
- Connection of fundamental results to U.S.-China Clean Energy Research Center focus areas involving engine tests

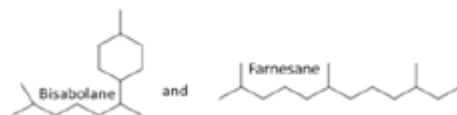


Figure 6. Structures of bisabolane and farnesane.

### References:

- [1] Peralta-Yahya P. P.; Ouellet M., Chan, R. Mukhopadhyay, A. Keasling, J.D. Lee, T. S. *Nature Communications* 2011, 2, 483.
- [2] Fisher, E.M.; Pitz, W.J.; Curran, H.J.; Westbrook, C.K. *Proc. Combust. Inst.* 2000, 28, 1579.
- [3] Dooley, S.; Curran, H. J.; Simmie, J.M. *Combust. Flame* 2008, 153, 2.



## Advanced Biofuels and Clean Combustion

## In-Cylinder Biofuel Combustion Behavior

Joint Project

## China Research Team Lead

- Mingfa Yao, Tianjin University

## China Partners

- Tianjin University

## Research Objective

The project is characterizing the performance, combustion, and emissions of n-butanol fuel/biodiesel dual-fuel high premixed compression combustion (HPCC).

## Technical Approach

- Conduct an experimental and modeling study of biodiesel surrogate combustion in a compression-ignition (CI) engine
  - Identify an appropriate biodiesel substitute for CI engine applications and prove its effectiveness as a surrogate
  - Develop a reduced chemical kinetics mechanism of biodiesel
  - Simulate biodiesel combustion using a coupled multidimensional computational fluid dynamics (CFD) model with the above reduced mechanism
- Conduct an experimental study on performance and emissions of a CI engine fueled with n-butanol/biodiesel in dual-fuel mode
  - Investigate the effects of n-butanol fuel rate, biodiesel injection timing, and exhaust gas recirculation (EGR) rate on dual-fuel HPCC

## Significant Results

Experimental and modeling study of biodiesel surrogate combustion in a CI engine: This work concerns the oxidation of biodiesel surrogates in a CI engine. The project team conducted an experimental study in a single-cylinder common-rail CI engine with soybean biodiesel and two biodiesel surrogates containing neat

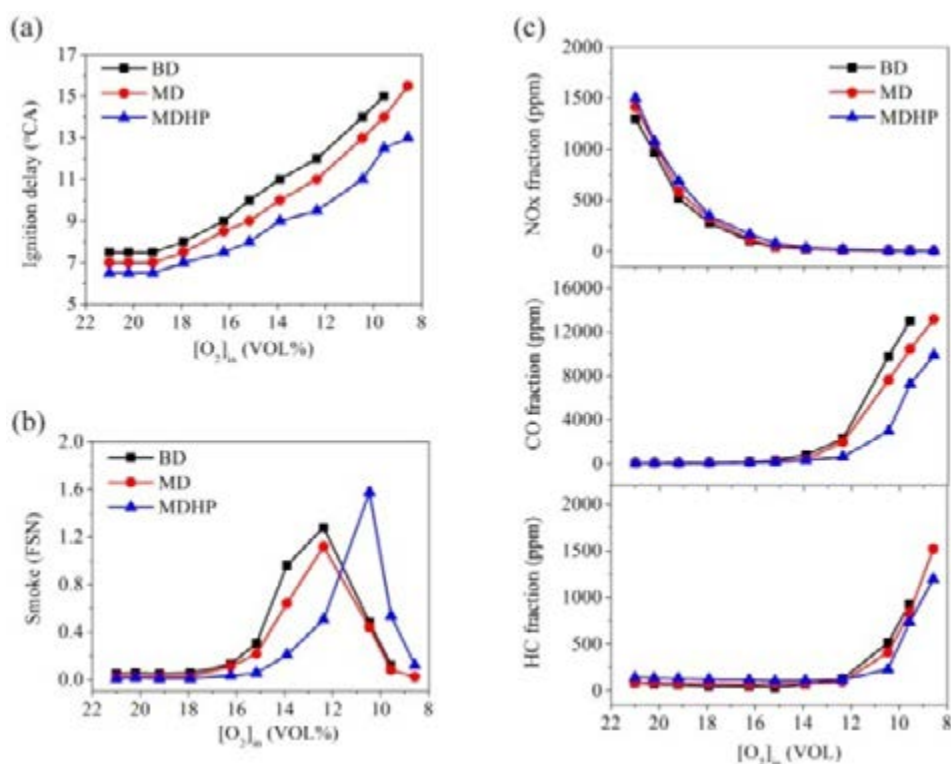


Figure 1. At the intake temperature of 25°C, the ignition delay and primary emissions of biodiesel (BD), methyl decanoate (MD), and methyl decanoate/n-heptane (MDHP) blends: (a) comparison of ignition delay; (b) comparison of smoke emission; and (c) comparison of CO, HC, and NOx emissions.

methyl decanoate and methyl decanoate/n-heptane blends. Tests were conducted with various intake oxygen concentrations ranging from 21% to approximately 9% at intake temperatures of 25°C and 50°C. Researchers compared the ignition delay and smoke emissions of neat methyl decanoate and methyl decanoate/n-heptane blends; results indicated that neat methyl decanoate was more similar to soybean biodiesel.

Researchers have developed a reduced chemical kinetic mechanism for the oxidation of methyl decanoate and applied it to model internal combustion engines. The computational platform was a KIVA code,<sup>1</sup> coupled with the Chemkin chemistry solver. Decreasing the intake oxygen concentration from 21% to 10.4% delayed the OH emission, and the OH distribution zone changed from near the anterior part of the spray to around the spray. As the intake oxygen concentration decreased from 21% to 12.4%, the soot emission increased. However, with the intake oxygen concentration at 10.4%, the soot emission was lower than the peak value.

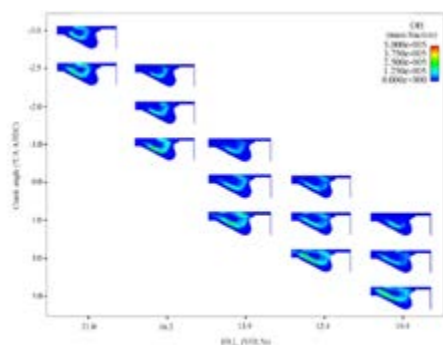


Figure 2. OH concentration distribution when autoignition occurs.

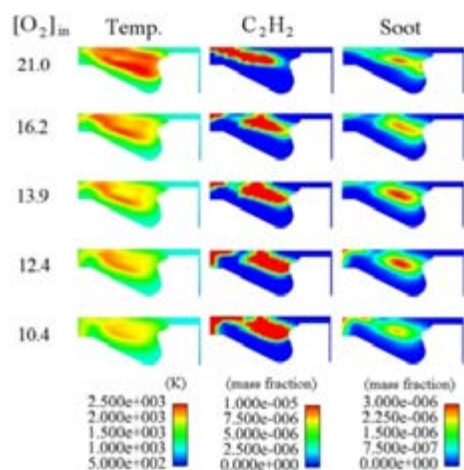


Figure 3. In-cylinder images of the distribution of temperature,  $C_2H_2$ , and soot at CA50 (crank angle for 50% heat release).

*An experimental study on the combustion performance and emission characteristics of n-butanol/biodiesel dual-fuel HPCC:* With the proper timing and ratio of biodiesel direct injection and n-butanol port injection, HPCC is achieved. The project team studied a range of influences on HPCC and emissions, including the rail pressure of biodiesel fixed at 100 megapascals, the circulating fuel consumption fixed at 60 milligrams (equivalent to biodiesel cycle consumption), the n-butanol ratio, biodiesel injection timing, and EGR rate. The results indicated that n-butanol ratio, EGR rate, and biodiesel injection timing affect HPCC and emissions through the cylinder mixture's charge stratification and the chemical reactivity stratification. HPCC is a compound combustion model comprising multicomustion styles; varying the biodiesel start of injection, EGR rate, and n-butanol ratio can achieve HPCC's ultra-low NOx and smoke paired with high efficiency. The project team found that the indicated thermal efficiency reaches 47% while NOx and soot emissions remain low when the EGR rate is set at 40%, the n-butanol ratio is set at 85%, and biodiesel injection timing is approximately -30°CA after top dead center (ATDC).

#### Future Plans

The project team is developing a reduced chemical kinetics mechanism of n-butanol/biodiesel blends. Coupling the reduced mechanism with a multidimensional CFD model, researchers will simulate HPCC. They will investigate the potential of HPCC with biofuel for load expansion and emissions reduction.

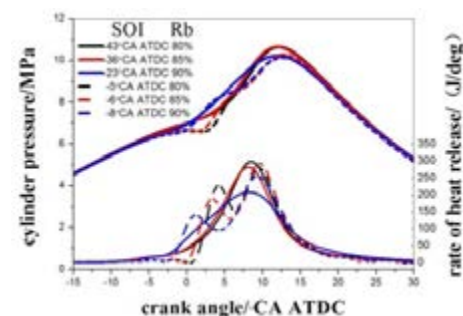


Figure 4. Combustion performance for different starts of injection (SOI) and n-butanol ratios (Rb).

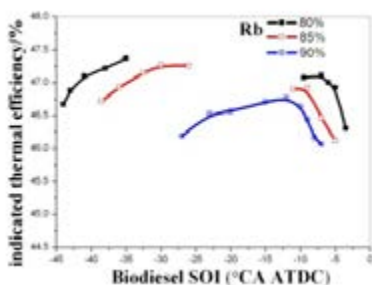


Figure 5. Indicated thermal efficiency of different SOI and Rb.

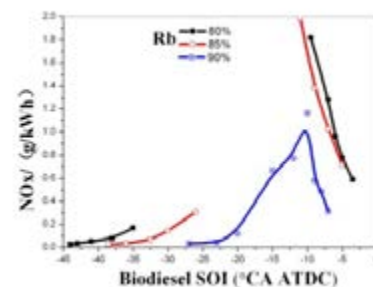


Figure 6. NOx emissions of different SOI and Rb.

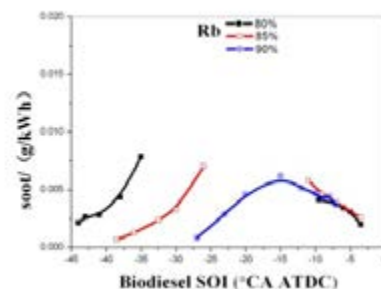


Figure 7. Soot emissions of different SOI and Rb.

#### Expected Outcomes

An understanding of advanced and novel combustion modes and a validated CFD model with coupled chemistry to guide engine design for operation with n-butanol/biodiesel dual-fuel or blending mode

- Detailed fundamental knowledge to support HPCC system optimization for high-efficiency and clean engines

<sup>1</sup> Los Alamos National Laboratory is developing KIVA, a transient, three-dimensional, multiphase, multicomponent code for the analysis of chemically reacting flows with sprays.

## Advanced Biofuels and Clean Combustion

# Integrated Powertrain and Aftertreatment System Control for Clean Vehicles

Joint Project

U.S. Research Team Lead	China Research Team Lead
<ul style="list-style-type: none"> <li>Junmin Wang, The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>Fuyuan Yang, Tsinghua University</li> </ul>
U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>The Ohio State University</li> <li>University of Michigan</li> <li>Oak Ridge National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> <li>Shanghai Jiao Tong University</li> </ul>

## Research Objective

The objective of this project is to develop synergistically integrated, systematic, optimal, and generalizable control methodologies for clean vehicle (CV) powertrain systems. Such control systems will optimally coordinate fuel property estimation, advanced combustion modes, exhaust aftertreatment systems, and hybrid powertrains to enable maximization of the energy efficiency and emission reduction potentials for CVs.

## Technical Approach

- Develop a fuel property adaptive engine control strategy
- Establish transient control methods for advanced combustion engines with consideration for fuel property uncertainties
- Create integrated and optimal engine, aftertreatment, and hybrid powertrain control methods

## Significant Results

The project team has developed a method to estimate fuel properties using high-pressure common rail pressure signals for diesel engines. Figure 1 shows the simulated rail pressure signals of different fuels in the frequency domain, clearly demonstrating differences among different fuels.

- Developed a control-oriented, multiphase combustion model applicable for diesel and biodiesel fuels in diesel engines. The premixed and mixing-controlled combustion is modeled by using two cascaded Wiebe functions. A set of Wiebe coefficients, which are partially physics-based, is found through a grey-box parameter identification approach
- Developed an ignition-delay correlation and CA50 prediction models applicable for diesel and biodiesel fuels. Figure 2 displays the comparison of model-predicted and measured CA50 for both B0 and B100 fuels. The model-predicted values match well with experimentally measured values

The team produced several publications during this reporting period:

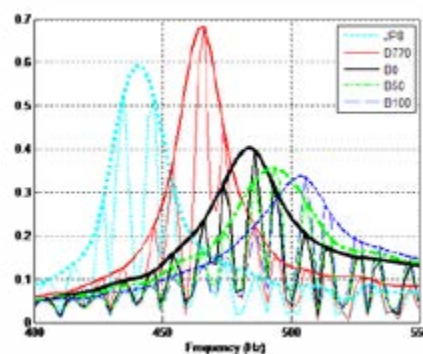


Figure 1. Simulated rail pressure signals and their envelopes for different fuels.

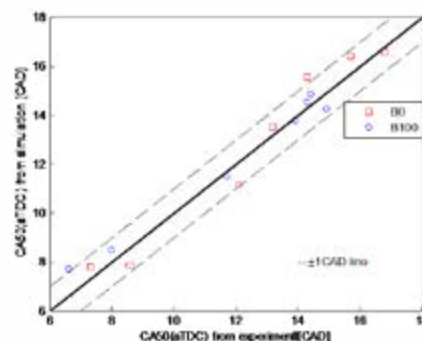


Figure 2. Comparison of model-predicted and measured CA50 for both B0 and B100 fuels (biodiesel fuel blends).

- Junfeng Zhao and Junmin Wang. "Control-Oriented Multi-Phase Combustion Model for Biodiesel Fueled Engines." *Applied Energy* 108 (2013): 92–99
- Junfeng Zhao and Junmin Wang. "Effect of Exhaust Gas Recirculation on Biodiesel Blend Level Estimation in Diesel Engines." *ASME Transactions Journal of Dynamic Systems, Measurements, and Control*, 135(1), 011010 (October 30, 2012) (7 pages)

- Junfeng Zhao and Junmin Wang. "On-Board Fuel Property Identification Method Based on Common Rail Pressure Signal." *Proceedings of the 2012 ASME Dynamic Systems and Control Conference* (invited paper), 2238-2245
- Junfeng Zhao and Junmin Wang. "Energy-based and Oxygen-based Biodiesel Blend Level Estimation Methods for Diesel Engines." *Proceedings of the 2012 American Control Conference* (invited paper), 4975-4980

## Future Plans

The project team will continue its efforts toward developing fuel property adaptive engine control methods, engine NOx emission control strategies with respect to fuel property variations, and integrated powertrain and aftertreatment system control methodologies.

Real-time control and estimation algorithm implementations and engine experiments will be further conducted to gather experimental data to evaluate the effectiveness of the proposed methods.

To support these efforts, mutual visits between U.S. and Chinese research partners for collaborative research activities will continue.

## Expected Outcomes

- Adaptive engine control methodologies for maintaining optimal engine performance with uncertainties in fuels and consideration of advanced combustion modes
- A framework for integrated engine, aftertreatment, and hybrid powertrain system control method development
- Understanding of the powertrain control system design requirements for different configurations and markets



## Advanced Biofuels and Clean Combustion

## Development of APU-Oriented Boxer Engine

Cooperative Project (China)

## China Research Team Lead

- Min Xu, Shanghai Jiao Tong University

## China Partner

- Shanghai Jiao Tong University

*Research Objective*

This project is developing a small displacement boxer engine that will be used as a special auxiliary power unit (APU) engine. The boxer engine has the advantages of a low fuel consumption rate; low noise, vibration, and harshness (i.e., high noise, vibration, and harshness [NVH] performance); a light weight; and an extremely compact structure. The ultimate goal is to develop and produce a prototype boxer engine.

*Technical Approach*

- Develop a small displacement boxer engine as an APU-specific engine by accomplishing the following:
- Develop an engine concept design
- Analyze subsystems
- Use computer-aided design (CAD) to optimize components
- Validate these elements using computer-aided engineering (CAE)
- Optimize the structure
- Test the resulting products

*Significant Results*

To study the design of two-stroke, horizontally opposed direct-injection engines, the project team completed benchmark testing for three engines: a 0.5-liter unmanned aerial vehicle two-stroke engine, a two-cylinder horizontally opposed engine from BMW, and a gasoline direct-injection engine from Volkswagen 1.4TSI.

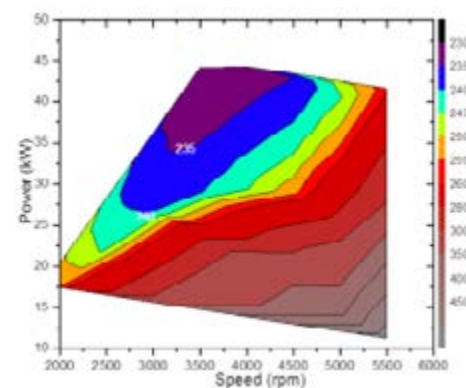
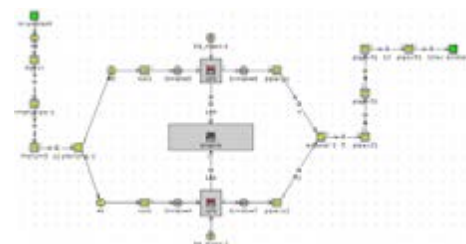
To consider the intellectual property problem and main design challenges, the researchers analyzed dozens of patents for horizontally opposed boxer engines and more than 400 SAE papers.

In accordance with the project plan, the APU-oriented boxer engine concept design and layout design have been developed. Also complete are geometric three-dimensional designs of intake/exhaust systems, cooling systems, crankshaft systems, lubrication systems, and combustion systems, including the one-dimensional performance and NVH simulation. Detailed three-dimensional computational fluid dynamics (CFD) and structure simulation work is ongoing.

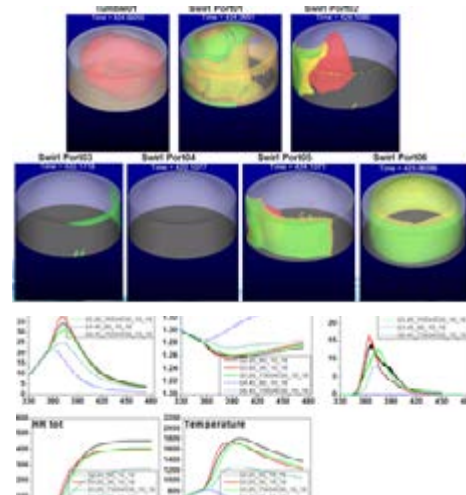


Researchers are using forward engineering in this project. During the concept design, they established one-dimensional simulation models of the engine performance and structure dynamics. To obtain the engine's key parameters to satisfy the research goal, the project team used the engine thermodynamics model provided by GT-POWER, U.S. Department of Energy analyses of multiple parameters, the Kriging fitting method, and genetic algorithm optimization. Examples of such parameters include port size, scavenging opening size, engine displacement, and compression ratio.

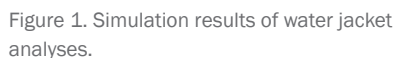
After determining some of these key parameters, researchers carried out a CFD analysis of the combustion system to validate the CAD design and to optimize the detail design process. This analysis consisted of three parts: (1) analysis of the scavenge process, (2) in-cylinder conduct of a detailed spray arrangement (with special attention paid to the total mass of wall film caused by impingement of spray droplets), and (3) combustion simulation. The team investigated details of the combustion form ignition to complete burn out to determine different structures of the scavenging port design. The project team ultimately accepted Plan 2 for a swirl-type scavenging port.



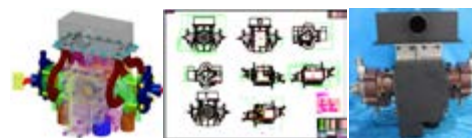
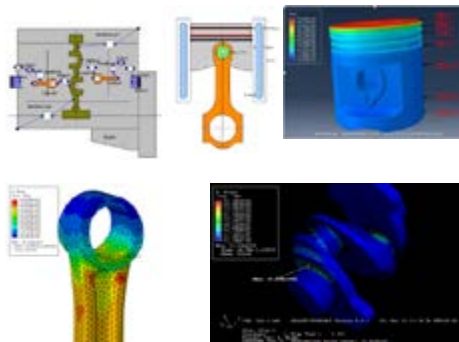
To ensure good performance and economy, it is very important that the engine work in an acceptable temperature range. To provide for proper engine cooling, researchers conducted a three-dimensional CFD analysis focused on the water jacket structure, identifying the number



The team also conducted some structural analyses to enable a more detailed design process. A lumped mass method was applied to check the strength of the main shaft bearings. Also, researchers used the Reynolds function



After completing all system analyses, the project team developed detailed designs for the components of each system, then processed the components. Finally, the project team successfully designed and assembled a sample engine.



Researchers will continue conducting tests with a focus on component optimization. They will also work toward developing a control strategy, considering features such as driving and electricity supply modules, ignition controls, and spray control.

- CAD model of a boxer engine and a CAE analysis report
- Prototype boxer engine
- Testing report
- Optimized engine control strategy



## Advanced Biofuels and Clean Combustion

## APU-Oriented High Efficiency and Clean Combustion System

Cooperative Project (China)

## China Research Team Lead

- Jianxin Wang, Tsinghua University

## China Partners

- Tsinghua University

## Research Objective

The objectives of this project are to understand the knocking mechanism that results from a pressure wave being coupled with a chemical reaction, evaluate the effect of high exhaust concentration on compression ignition and knocking, and identify new approaches to suppress knocking.

## Technical Approach

- Determine flame characteristics and pressure waves during knocking using an optical engine
- Investigate pressure oscillation and chemical kinetics coupling during knocking combustion using computational fluid dynamics (CFD) with chemical kinetics

## Significant Results

The main results of this project include determining flame characteristics and evaluating pressure wave and chemical kinetics coupling.

The knocking phenomenon has been an inherent problem of internal combustion engines from their inception. It is the main obstacle toward increasing the compression ratio to improve the thermal efficiency of spark ignition (SI) engines. In recent years, engine knock has been studied intensively with an eye toward energy savings, especially in light of rapid progress in combustion diagnostics and chemical kinetics that enables improved understanding of this complicated combustion process.

**Flame characteristic and pressure wave investigation using an optical engine:** As shown in Figure 1, the autoignition process of the end gas area near the cylinder wall was captured using a top view optical engine with a compression ratio of 14. Compared with the pressure trace, the images indicate more clearly whether and how the autoignition of these small hot spots transition into a runaway knocking.

Using the same engine but with a metal cylinder head (Figure 2), different knocking induction mechanisms and pressure wave propagation

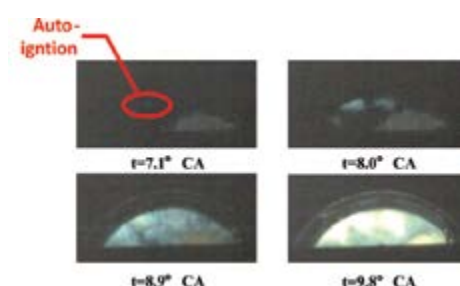


Figure 1. Flame propagation and autoignition.

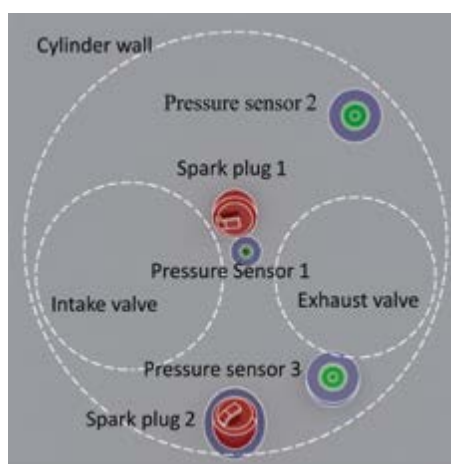


Figure 2. Cylinder head used to investigate super-knock.

processes were investigated. The pressure wave oscillation modes and onset time were calculated from the pressure traces (Figure 3) obtained from different locations to help understand the physical nature of knocking.

**Pressure oscillation and chemical kinetics coupling study using CFD models:** To more fully understand the physical-chemical mechanism

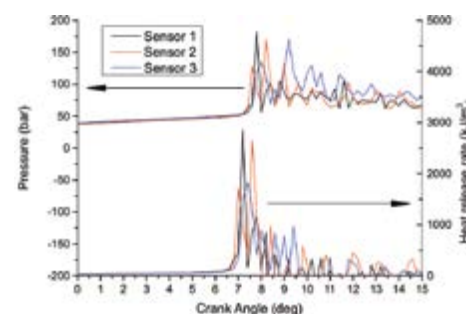


Figure 3. Pressure waves of knocking combustion.

during knocking combustion and the deflagrative flame structure, the project team had to consider complex chemical kinetics and pressure wave propagation phenomena, as well as their interactions. Team members investigated pressure wave and intermediate species interactions during knocking combustion using a G-equation flame propagation model with a chemistry mechanism that includes aldehydes such as  $\text{CH}_2\text{O}$  and radical species such as  $\text{HCO}$  to indicate autoignition. The CFD predictions are analyzed together with the cylinder pressure and combustion visualizations to understand their dynamic interactions.

As Figure 4 shows, the heat release peak is in phase with the pressure wave peak, and the Rayleigh Index (RI) is positive and maximized at  $8.74^\circ\text{CA}$ . The duration of positive RI is short (about  $0.1^\circ\text{CA}$ ). Even a short period with  $\text{RI} > 0$  can excite the combustion wave near the wall. This leads to high-frequency pressure

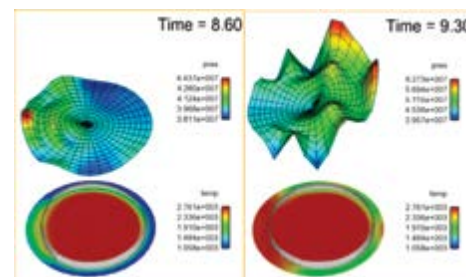


Figure 4. Two representative timings of autoignition in the mid-plane of the cylinder.

oscillations in the high-temperature gas near the wall. Because the unburned mixture is distributed near the wall in SI engines, the interaction of pressure waves and the chemical reaction usually occurs near the wall in knocking combustion.

Combustion in compression ignition engines typically has larger amplitude pressure oscillations than combustion in SI engines. However, the pressure waves in diesel engines or homogeneous charge compression ignition engines typically do not result in engine damage, because diesel engines have lower maximum temperatures and no unburned rich mixture near the wall to promote thermoacoustic coupling.

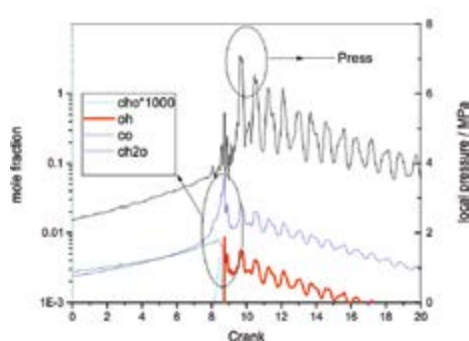


Figure 5. Local pressure waves, heat release rates, and Rayleigh Index.

### Future Plans

The project team will study the effects of internal and external exhaust gas recirculation on combustion stability, thermal efficiency, and particulate matter emissions. Researchers will investigate the ignition mechanism and combustion stability in diluted conditions using a stratified stoichiometric mixture with two-zone homogeneity. Phase compensation will be used to study knock characteristics and suppression methods.

### Expected Outcomes

- New proposed knock suppression methods
- Design schemes and control criteria of two highly efficient, low-emission combustion systems

## Advanced Biofuels and Clean Combustion

## Integration and Systematic Control of APU System

Cooperative Project (China)

U.S. Research Team Lead	China Research Team Lead
• Junmin Wang, The Ohio State University	• Fuyuan Yang, Tsinghua University
U.S. Partners	China Partners
• The Ohio State University	• Tsinghua University

*Research Objective*

The objective of this project is to reduce engine emissions substantially by developing a control technology for a low-temperature combustion (LTC) auxiliary power unit (APU). An optimized APU system and control strategy will improve APU efficiency and reduce vehicle emissions. LTC in part engine load conditions will take advantage of the high-pressure common rail system's exhaust gas recirculation and variable nozzle turbine.

*Technical Approach*

- Develop an automatic switching control method between LTC mode and conventional compression ignition (CI) combustion
- Conduct simulation research on APU system energy management
- Apply in-cycle combustion feedback control to reduce cycle-to-cycle variation

*Significant Results*

LTC has limited operation range. The project team developed automatic switching control technology between LTC and CI to apply LTC in diesel engines in a practical way. Coordinating control of fuel and air systems enabled smooth switching between the two different combustion modes, LTC and CI.

The project team established a simulation model of APU system energy management, basing the model on a range-extended electric bus and using the driving cycle of a city bus in China. Researchers tested the performance of two different energy management strategies, charge-depleting charge-sustaining (CDCS) and blended. The simulation results show that, for the system constructed in the project, CDCS is superior to blended.

The team also investigated accurate combustion control, which can be achieved through in-cycle combustion feedback control. Such

control enables feedback signal collection, algorithm execution, and control parameter adjustment in one engine cycle. The project team developed a two-core engine control unit, with one core for engine control and the other for cylinder pressure processing. Researchers developed an online Start of Combustion (SOC) detection method based on motored cylinder pressure estimation. Taking SOC as a feedback signal and main injection timing as a control parameter, the research team developed an in-cycle combustion feedback control algorithm. Experimental results show that this method can improve the cycle-to-cycle variation of diesel engines.

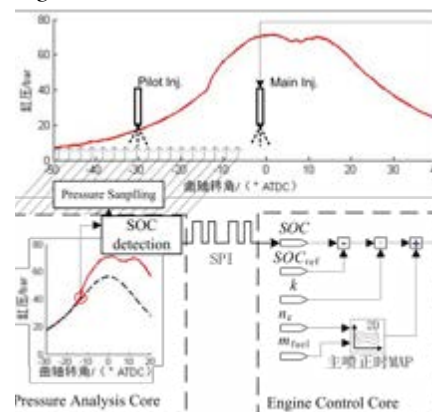


Figure 1. Control logic diagram of in-cycle combustion feedback control.

In addition to the efforts above, the team has published two papers:

- Fuyuan YANG, Guojing GAO, Minggao OUYANG, Lin CHEN, and Yuping YANG. "Research on a diesel HCCI engine assisted by an ISG motor." *Applied Energy* 101 (2013): 718-729
- Guojing GAO, Fuyuan YANG, Lin CHEN, Yuping YANG, and Minggao OUYANG. "Transient control of low-temperature premixed combustion using ISG motor dynamic torque compensation." 2012 IEEE Vehicle Power and Propulsion Conference, October 9–12, 2012

*Future Plans*

The project team plans to study optical control of diesel combustion based on combustion mode identification. The team will also do experimental testing of APU systems and validation of APU control strategies.

*Expected Outcomes*

- An integrated APU control system
- An APU prototype and automatic switching control method between homogeneous charge compression ignition and CI
- A coordination control algorithm of an engine and generator and an optimized APU energy management strategy

## Advanced Biofuels and Clean Combustion

## Energy Conversion

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• University of Michigan</li> <li>• The Ohio State University</li> <li>• Oak Ridge National Laboratory</li> <li>• Sandia National Laboratories</li> </ul>	<ul style="list-style-type: none"> <li>• Wuhan University of Technology</li> </ul>

## Research Objective

The objective of this project is develop novel, highly efficient, and inexpensive nanocomposite thermoelectric materials with dimensionless figure of merit (ZT)  $\sim 1.5$  to convert waste heat of cars and trucks into electricity. The project will also determine a Seebeck coefficient using scanning thermoelectric microscopy (SThEM) in conjunction with scanning tunneling microscopy to measure sample homogeneity on a nanometer scale.

## Technical Approach

- Seek a high Seebeck coefficient and high electrical conductivity while simultaneously aiming for as low a thermal conductivity as possible. To achieve this, explore the formation of band-resonant states in nanocomposite materials such as  $\text{CoSb}_3$ -based skutterudites and various forms of doping  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions

## Significant Results

The main results of this project so far include the development of antimony (Sb)-doped n-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions with  $\text{ZT} = 1.35$ , and the development of operational scanning Seebeck coefficient microscopy.

In addition, the research team has published several joint publications supported by the U.S.-China Clean Energy Research Center Clean Vehicles Consortium program:

- W. Liu, X. F. Tang, H. Li, J. Sharp, X. Zhou, and C. Uher. "Optimized Thermoelectric Properties of Sb-doped  $\text{Mg}_{2(1+z)}\text{Si}_{0.5-y}\text{Sn}_{0.5-y}\text{Sb}_y$  Through the Adjustment of Mg Content." *Chemistry of Materials* 23, 5256 (2011)
- W. Liu, X. Tan, K. Yin, H. Liu, X. F. Tang, J. Shi, Q. Zhang, and C. Uher. "Convergence of Conduction Bands as a Means of Enhancing Thermoelectric Performance of N-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  Solid Solutions." *Physical Review Letters* 108, 166601 (2012)
- W. Liu, X. F. Tang, H. Li, K. Yin, J. Sharp, X. Zhou, and C. Uher. "Enhanced Thermoelectric Properties of N-type  $\text{Mg}_{2.16}(\text{Si}_{0.4}\text{Sn}_{0.6})_{1-y}\text{Sb}_y$  due to Nano-sized Sn-rich Precipitates and an Optimized Electron Concentration." *Journal of Materials Chemistry* 22, 13653 (2012)
- X. J. Tan, W. Liu, H. J. Liu, J. Shi, X. F. Tang, and C. Uher. "Multiscale Calculations of Thermoelectric Properties of N-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  Solid Solutions." *Physical Review B* 85, 205212 (2012)
- W. Liu, K. Yin, X. Su, H. Li, Y. Gao, X. F. Tang, and C. Uher. "Enhanced Hole Concentration Through Ga Doping and Excess of Mg and Thermoelectric Properties of P-type  $\text{Mg}_{2(1+z)}(\text{Si}_{0.3}\text{Sn}_{0.7})_{1-y}\text{Ga}_y$ ." *Intermetallics* 32, 352 (2013)
- X. J. Tan, H. J. Liu, J. Wei, J. Shi, X. F. Tang, and C. Uher. "Thermoelectric Properties of Small Diameter Carbon Nanowires." *Carbon* 53, 286 (2013)

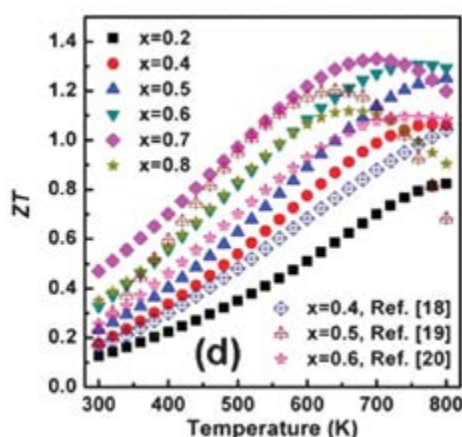


Figure 1. Dimensionless thermoelectric figure of merit (ZT) of n-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions.

## Future Plans

The initial attempt to form bond resonant states with tin (Sn) doping in  $\text{CoSb}_3$  will be followed with other prospective dopants to further improve the Seebeck coefficient of  $\text{CoSb}_3$ -based skutterudites.

The research team will attempt to improve the performance of n-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions by doping with bismuth, which is a heavier element. A greater mass difference in comparison to antimony-doped structures should result in lower lattice thermal conductivity and thus higher ZT.

The research team will also focus on improving the performance of p-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions that, so far, lag far behind the n-type forms of the material.

Modifications will be made to a sample holder of the SThEM apparatus to allow measurements of thin-film samples.

## Expected Outcomes

- Development of high-performance p-type skutterudites for waste heat recovery
- Development of efficient and inexpensive n-type  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions
- Improvement of p-type forms of  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$
- Development of low-resistance contacts to both forms of  $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$  solid solutions
- Implementation of scanning Seebeck coefficient microscopy for nanometer-scale characterization of dopant distribution in thermoelectric materials



## Vehicle Electrification

## Efficient and High Power Density Electric Powertrain

Joint Project

U.S. Research Team Lead	China Research Team Lead
<ul style="list-style-type: none"> <li>• Heath Hofmann, University of Michigan</li> <li>• Longya Xu, The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>• Wen Xuhui, Chinese Academy of Sciences</li> <li>• Tao Fan, Chinese Academy of Sciences</li> </ul>
U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• University of Michigan</li> <li>• The Ohio State University</li> <li>• Oak Ridge National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>• Chinese Academy of Sciences</li> <li>• Jing-Jin Electric</li> <li>• Hunan CSR Electric Vehicle Company</li> </ul>

*Research Objective*

This project will seek to develop innovative and optimized electric machines to achieve an electrified powertrain with significantly higher power density and efficiency. This will be achieved through the investigation of novel electric machine designs and the development of computationally efficient design tools.

*Technical Approach*

- Develop computationally efficient yet accurate steady-state analysis techniques for finite element models of electric machines
- Develop innovative electric machine topologies that are integrated with vehicle transmissions
- Reduce machine losses so that air cooling becomes feasible, dramatically increasing the power density of the overall system

*Significant Results*

Researchers at the University of Michigan have created and improved two separate steady-state analysis techniques for electric machines. One, the Shooting-Newton Method, has been shown to work best with current-driven models. The other, Harmonic Balance, has been shown to work best with voltage-driven models. Both of these techniques are included in the first version of the electric machine simulation software. This software is now available for download through the University of Michigan CTools website. This accessibility will provide an opportunity for industry partners and the other project members performing machine design to provide feedback on the tool and request new features. In turn, this will help guide the development of future algorithms that will be of the most benefit to the project.

Researchers at the Chinese Academy of Sciences have optimized the design of a permanent magnet machine with amorphous iron laminations. A prototype of this design was built and compared to a design with conventional silicon laminations. The high-frequency capability of the amorphous iron material allowed for a significant increase in efficiency (as much as five percentage points) over the conventional machine. The prototype

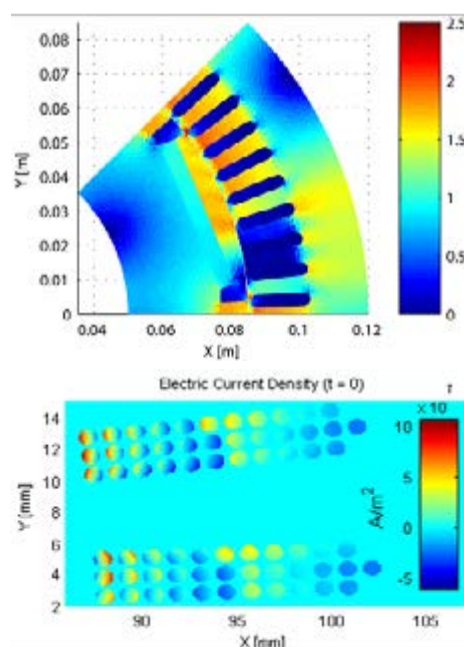


Figure 1. Top: Flux density distribution in interior permanent magnet machine. Bottom: Current density distribution in two slots of a two-layer electric machine winding with stranded conductors due to proximity effect.

machine is also significantly smaller than the conventional machine.

Publications related to this work over the past year include the following:

- J. Pries and H. Hofmann. "Steady-state finite element analysis of magnetic devices using a shooting-Newton/GMRES algorithm with Runge-Kutta integration," in proceedings of the Energy Conversion Congress and Exposition (ECCE), 2012 IEEE
- Q. Li, T. Fan, and X. Wen. "Armature-Reaction Magnetic Field Analysis for Interior Permanent Magnet Motor Based on Winding Function Theory." *IEEE Transactions on Magnetics* 49(3) (March 2013): 1193-1201

*Future Plans*

Researchers at the University of Michigan are currently developing a steady-state simulation algorithm that is suitable for parallel computation. An 80-core, high-performance computer has been acquired to aid in this development. They would also like to query research and industrial partners to see if there is an interest in the development of steady-state multiphysics algorithms (e.g., magnetic + thermal). It is believed that the steady-state techniques being pursued could dramatically reduce the simulation time of such problems.

*Expected Outcomes*

- Computationally efficient two- and three-dimensional steady-state solvers for synchronous and asynchronous machines
- High-efficiency machine designs that will eliminate the need for liquid cooling, thereby dramatically increasing power density and reliability
- A novel electrical variable traction-transmission design by real-time hardware-in-loop valuation
- Design rules aiming at trade-offs between harmonic core losses and harmonic power for saturated amorphous alloy permanent magnet machines



Figure 2. Left: Prototype amorphous iron stator core. Right: Completed machine.

## Vehicle Electrification

## Control and Optimization of Distributed Vehicle Network

Joint Project

U.S. Research Team Lead	China Research Team Lead
• Junmin Wang, The Ohio State University	• Jianqiu Li, Tsinghua University
U.S. Partners	China Partners
• The Ohio State University	• Tsinghua University

*Research Objective*

The objective of this project is to deal with the motion dynamics control of four-wheel independent-drive electric vehicles (4WID-EVs) with networked control systems and to improve the control robust against controller area network (CAN)-induced time-varying delays.

*Technical Approach*

- Establish the control-oriented model for vehicle lateral dynamics with network-induced time delays
- Express the network time delay uncertainties with matrix polytope
- $H^\infty$ -based linear-quadratic regulator tracking control is obtained and solved in the form of a sequence of linear matrix inequalities (LMIs) for the control synthesis
- The whole controller design process is shown in Figure 1

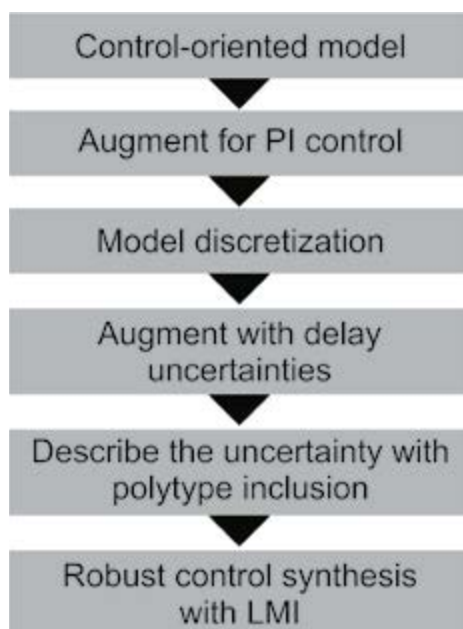


Figure 1. Controller design process.

*Significant Results*

The main results of this project are shown in Figures 2 and 3. Clearly, once there are network time-varying delays in the closed loop, the yaw rate of the vehicle controlled by the conventional controller oscillates significantly after a non-zero steering wheel angle trigger, while the project's proposed controller demonstrates good robustness against the CAN-induced network time-varying delays.

*Future Plans*

Future work will address the state estimation problem of 4WID-EVs with networked control systems. The team will also investigate fault diagnosis and fault-tolerant control of 4WID-EVs with networked control systems.

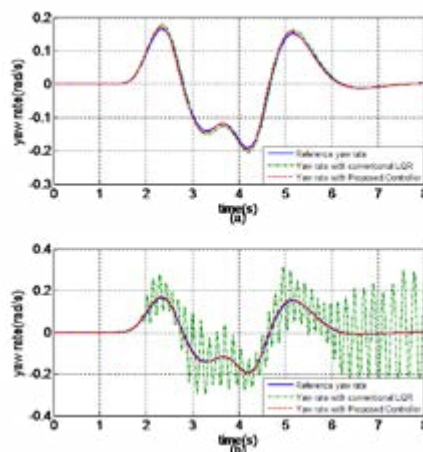


Figure 2. Vehicle yaw rate response in a double lane-changing maneuver (a) under ideal network conditions and (b) with CAN-induced delays.

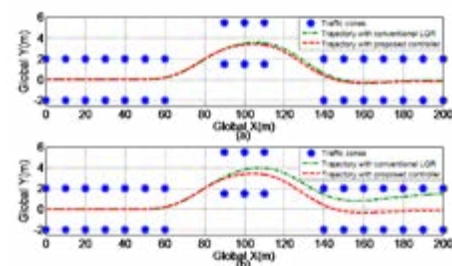


Figure 3. Vehicle center-of-gravity trajectory in a double lane-changing maneuver (a) under ideal network conditions and (b) with CAN-induced delays.

*Expected Outcomes*

- A full set of network control algorithms for vehicle dynamics of 4WID-EVs

## Vehicle Electrification

# Rapid System Integration through Modular Configuration, Sizing, and Control for Hybrid Vehicles

Joint Project

U.S. Research Team Lead	China Research Team Lead
<ul style="list-style-type: none"> <li>Huei Peng, University of Michigan</li> <li>Jing Sun, University of Michigan</li> <li>Giorgio Rizzoni, The Ohio State University</li> <li>Simona Onori, The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>Jianqiu Li, Tsinghua University</li> <li>Chengliang Yin, Shanghai Jiao Tong University</li> </ul>
U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Michigan</li> <li>The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> <li>Shanghai Jiao Tong University</li> </ul>

## Research Objective

The project is developing key techniques for the modeling, analysis, design, and control of power-split hybrid vehicles.

## Technical Approach

- Perform analysis and automated modeling of all configurations of power-split hybrid vehicles with multiple operating modes
  - Study powertrains that use a single planetary gear
  - Expand to powertrains using two planetary gears
- Develop modeling and optimization methods that enable rapid computation of control algorithms for powertrains with multiple modes
- Focus on specific applications to accelerate technology transfer

## Significant Results

The project team has designed and analyzed the conceptual “Prius+” and “Volt-” vehicles that are similar to the two popular production hybrid vehicles but were obtained after an exhaustive search of all possible configurations and optimal control, including all possible operation modes. As an example, using the lever diagram analogy, the Prius powertrain is represented by the diagram shown in Figure 1. It deploys no clutch and only one mode. After thorough topological analysis, researchers found that three clutches can be added to enable four operating modes. The additional modes were found to achieve better launching and fuel economy performance in urban cycles.

The team also developed a method of power-weighted efficiency analysis for rapid sizing; the method analyzes the losses of the powertrain by using the statistical information of the drive cycle. The process was designed to enable rapid sizing of power-split hybrid vehicles with multiple operating modes. This method was found to be about 12,000 times faster

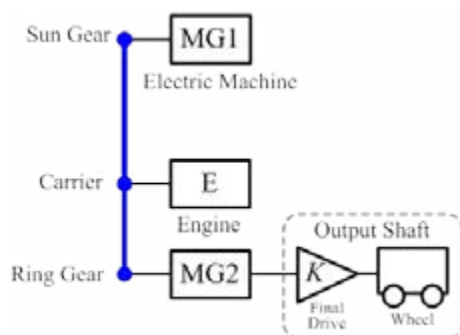


Figure 1. Original input-split configuration used in the Toyota Prius.

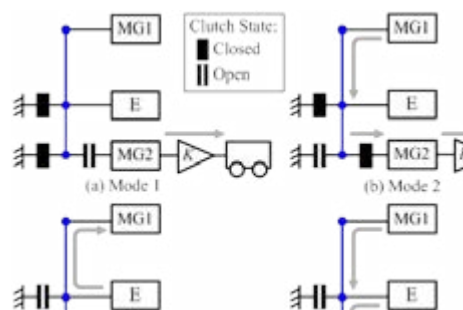


Figure 2. Enhanced input-split configuration with four modes: two electric vehicle modes, one serial mode, and one power-split mode.

than exhaustive optimization methods such as dynamic programs.

Using the automatic modeling and the rapid numerical method previously described, the project team analyzed all six input-split configurations. The researchers found that by adding clutches and operating modes and optimizing the component sizes, excellent vehicle fuel economy can be achieved while satisfying a given level of drivability assurance. In other words, many excellent design candidates can achieve world-class fuel economy

by taking advantage of all three degrees of freedom in powertrain design: configuration, sizing, and control (see Figure 3).

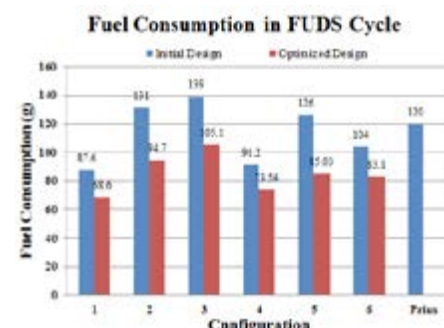


Figure 3. Fuel consumption results of optimal designs of all six input split-hybrid vehicles using a single planetary gear (federal urban driving cycle, or FUDS).

## Future Plans

The project team believes an important next step in the development of clean vehicles (CVs) is to push the envelope of key technologies that have already secured their successful commercial applications in light-duty applications to heavy vehicles for higher impacts. Certain power-split powertrains have captured 90% of the lightweight hybrid vehicle market share; these powertrains need to be further developed before use in heavy vehicle applications because of the much higher torque and power requirements. Powertrains using two planetary gears can have input split, compound split, fixed gear, electric vehicle, and electronically controlled variable transmission operations. Taking full advantage of these modes may necessitate clutches and multiple modes. The project team plans to fully analyze all 360 possible two-planetary-gear configurations and develop mode identification and automated modeling methods to create these configurations' dynamic models.

Subsequently, the team plans to explore high-potential CV applications, such as Class 3, 6, or 8 trucks, and to identify challenges such as limited battery energy and power/torque limitations. Also planned are studies of design challenges and potentials of alternative power-split powertrains, such as hydraulic hybrids, battery-assisted human powered vehicles (e-assisted bikes), etc. Again, these designs will fully explore configuration, sizing, and control for best performance.

#### *Expected Outcomes*

- Comprehensive modeling, analysis, and control tools for design and simulation of power-split vehicles using one or two planetary gears; two-planetary-gear designs are especially suitable for heavy-duty applications such as light trucks, sport utility vehicles, and trucks up to Class 6
- A complete study of the benefits and challenges in deploying clutches to enable multiple modes
- In-depth analysis of several powertrain designs for next-generation CV applications
- Technology transfer to U.S. industrial partners



## Vehicle Electrification

## Intelligent Fault Diagnosis and Prognosis

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>Hefei University of Technology</li> </ul>

*Research Objective*

The objective of this project is to develop methods, algorithms, and software tools for electrified vehicle diagnosis and prognosis to ensure safety, reliability, and longer life cycle. The current research objective is to develop a systematic methodology for the design of system-level diagnostics for the permanent magnet synchronous motor (PMSM) drive and system-level prognosis for the battery system. A future research objective is fault-tolerant control of the electric drive system to ensure limp-home capabilities in the event of failures.

*Technical Approach*

- Conduct hazard analysis (HA) including fault tree analysis and design failure modes and effects analysis for electrified powertrains
- Develop fault and aging models, including a novel aging propagation modeling approach for interconnected systems
- Develop simulators that permit fault injection and include aging models at the component level, as well as simulate their effects at the system level
- Develop system-level model-based state-of-health assessment and prognostics schemes for lifecycle management
- Develop fault-tolerant control strategies and algorithms for the electric drive system, as well as life extension strategies and algorithms for the battery system

*Significant Results*

**HA for electric vehicle (EV) powertrains:** The project team has successfully conducted HA for the electric drive system including the battery systems, power converter, and electric machine(s). The diagnostics and prognostics needs and challenges that have arisen with the introduction of electrified power trains were identified, and research directions were selected.

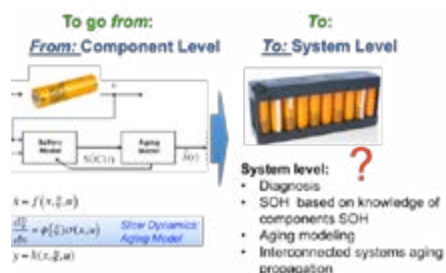


Figure 1. From battery cell to battery pack aging modeling.

**Fault and aging modeling:** Researchers have formulated mathematical models to be used in higher-level simulators to investigate the effects of component-level faults and aging on system-level performance. In particular, the project has developed the following:

- Mathematical models for the following types of faults in the PMSM drive system: a single-phase open-/short-circuit fault in the machine windings; an open/short circuit in the power switches
- Power and capacity fade models for lithium-ion battery cells
- A systematic methodology for modeling the propagation of aging in battery systems, based on the interaction between dynamic system models and dynamic models of aging

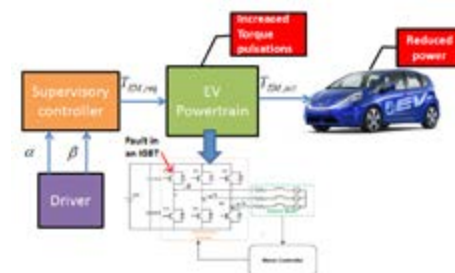


Figure 2. Forward-looking battery electric vehicle scheme for fault injection.

**Simulation tools development:** Using Matlab/Simulink, researchers have developed the following hierarchical simulation tools:

- A simulator for a battery electric vehicle including detailed models of the electric traction system, components, and corresponding faults

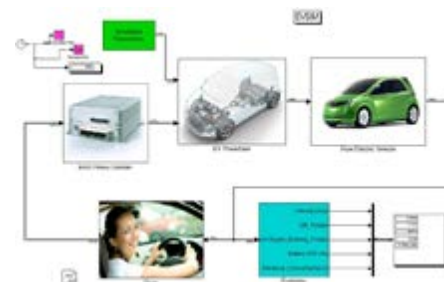


Figure 3. Snapshot of the battery electric vehicle simulator.

- A multi-time-scale battery pack simulator for aging propagation studies, accounting for electrical, thermal, and aging dynamics. The battery pack simulated is an air-cooled lithium-ion battery pack under 2P5S and 5S2P topologies. Aging at the cell level is modeled by coupling the electrical and thermal dynamics to the (slow) aging dynamics. Capacity and power fade were chosen as performance degradation (aging) metrics

**Industry and China collaboration:** The two teams have had highly profitable collaborations, including sharing of human capital and student exchanges, resulting in (among other results) development of the electric drive models and the fault models, thanks to a traveling researcher's expertise in electric machine control.

### *Future Plans*

The project team will conduct a deeper and more complete failure analysis for electric traction systems in collaboration with industry partners. The team also plans to develop model-based fault diagnosis and prognosis methods and procedures for EV electric drive systems. The methods and tools will be demonstrated on an experimental vehicle, again in collaboration with industrial partners.

### *Expected Outcomes*

- A systematic methodology for the design of system-level solutions for EV state-of-health assessment, diagnosis, and prognosis
- Methods, algorithms, and software tools for EV powertrain key systems life cycle management
- Fault-tolerant control methods for limp-home and life-extending operation of electrified powertrains
- Collaboration with U.S. and Chinese industry partners in implementing these methods and systems

## Vehicle Electrification

## Adaptive Battery Management System On and Off the Grid

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Michigan</li> </ul>	<ul style="list-style-type: none"> <li>Chinese Academy of Science</li> <li>Shanghai Jiao Tong University</li> <li>Tsinghua University</li> </ul>

*Research Objective*

This project seeks to develop intelligent monitoring (while driving), diagnosis/prognosis, and conditioning (while connected with the grid) strategies to improve the reliability, performance, and life cycle of battery systems on electrified vehicles. The current research objectives are directed toward the development of suitable models for battery system aging characterization and real-time adaptation, and the development of design framework and computational algorithms to perform robust battery system identification and diagnosis with onboard sensor and communication constraints.

*Technical Approach*

- Develop phenomenological models that can represent battery aging data while explaining underlying physical behavior
- Improve understanding of the aging and environmental effects on batteries' cycle performance
- Identify real-time and onboard battery system adaptation requirements and limitations
- Develop energy management algorithms and strategies to maintain optimal and robust performance for battery systems with changing characteristics

*Significant Results*

Efforts have been focused on characterization and identification of battery state of health (SOH) for electrified vehicles. The team has built a large database of battery aging cycles over the past two years. The data sets have been analyzed to develop/validate new models and SOH identification algorithms. The main results achieved so far include the design of an effective identification framework for onboard battery SOH monitoring and degradation diagnosis and the development of a unified battery open-circuit-voltage (OCV) model for state of charge (SOC) and SOH estimation.

The incremental capacity analysis (ICA) leverages the lithium-ion battery staging phenomenon during the intercalation process at the graphite anode side. This analysis exploits the sensitivity of the battery charged capacity (Q) with respect to the terminal voltage (V) and transforms voltage plateaus on the V-Q curve into clearly identifiable peaks on the dQ/dV curve. While it is known that the peaks on the incremental capacity (IC) curve are associated with battery electrochemical properties and aging status under quasi-equilibrium conditions, this project focuses on the investigation of the IC signature and its utility under normal charging conditions. Through extensive analysis of the aging data, a strong correlation is established between the IC peak at higher SOC range and the SOH for data collected under normal charging conditions (1/2 C rate).

Extracting the IC aging signatures from the battery charging/discharging data is challenging, as the flatness of the curve and the noise sensitivity make it infeasible to directly differentiate measured Q-V data. The team has

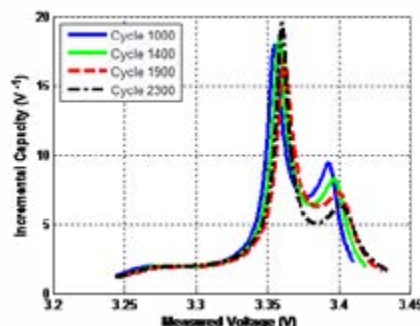


Figure 1. IC curves of data at different aging stages.

explored both parametric and non-parametric approaches, developed and evaluated several algorithms, and validated the algorithms with battery aging data sets. The use of support vector regression (SVR) is shown to provide the most promising features for real-time applications, because the SVR model is able to extract the IC peak information and predict the capacity fade within 1% error bound more than 90% of the time, as validated on data collected for eight different A123 LiFePO<sub>4</sub> cells with up to 2,800 aging cycles.

To complement the incremental capacity analysis (ICA)-based SOH monitoring, the project team proposes a new parametric OCV model that captures the staging phenomenon of the lithium-ion battery. Results show that the

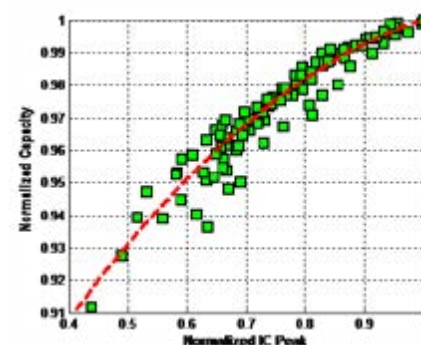


Figure 2. Correlation between normalized battery capacities and IC peaks.

new model improves SOC estimation accuracy compared to other existing OCV models, while providing the signature associated with aging to facilitate SOH monitoring.

*Future Plans*

Future research activities include the following: (1) augment the battery aging cycle data set to include tests for different temperatures, driving cycles, and operating conditions; (2) investigate

the sensitivity of the ICA-based SOH model to environmental and operational parameters (such as temperature and driving cycle); (3) characterize the influence of battery charging/discharging profiles on battery aging, as well as the associated effects on SOH monitoring and diagnosis; and (4) develop adaptive power management strategies incorporating battery SOH information.

#### *Expected Outcomes*

- Parametric models for battery system SOH monitoring and SOC identification
- Sensitivity analysis of battery system performance and aging behavior to charging/discharging patterns
- Algorithms and methodologies for online battery system identification and adaptation
- Validation and verification of an integrated off-grid/on-grid adaptive battery power management strategy
- Recommendations on battery system prognosis and diagnosis strategy



## Vehicle Electrification

## Data-Based Techniques for Battery-Health Prediction

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Michigan</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> </ul>

*Research Objective*

The objective of this project is to develop and demonstrate a noninvasive method to estimate health-relevant features of a battery and thus predict the battery's state-of-health (SoH). Unlike existing battery SoH estimation algorithms, the new approach will be data-based: a priori knowledge about the dynamics of the battery degradation mechanism will not be necessary. The developed algorithm will be validated using laboratory experiments.

*Technical Approach*

- Adopt the retrospective cost-based subsystem identification (RCSI) modeling technique to identify the dynamics of the battery health subsystem
- Develop a design approach for RCSI to capture the dynamic evolution of film growth on the anode at the solid-electrolyte interface (SEI), as the indicator of battery SoH
- Conduct simulations and laboratory experiments to validate the developed approach and evaluate its performance

*Significant Results*

The team formulated the battery SoH prediction problem as an inaccessible subsystem identification problem, with the RCSI technique as the solution approach. Simulations using high-fidelity models of battery electrochemistry dynamics showed that the proposed approach can accurately predict battery SoH by measuring the dynamic growth of the SEI film resistance. Figure 1 shows sample identification results, highlighting the performance of the algorithm. Note that the true evolution of the dynamics is not available in practice, but the estimates are. These results were published at the 2012 Dynamic Systems and Control Conference (DSCC).

The team is investigating the performance of the algorithm under measurement noise and model initialization errors to establish the conditions under which the algorithm will give reliable estimates. The preliminary results of this investigation are in review for publication at the 2013 DSCC.

*Future Plan*

- Use RCSI to find a larger portion of the health model
- Investigate impact of model uncertainty
- Use RCSI with laboratory cycling data
- Collaborate with the Chinese partners to support their battery state of function estimation activities
- Collaborate with the industry partners for technology transfer

*Expected Outcomes*

- A battery SoH prediction algorithm that works with noninvasive measurements and can be applied to different battery chemistries without requiring a priori knowledge of their degradation dynamics
- Design techniques for the algorithm to work under realistic conditions, including measurement noise and modeling errors
- Validation of the algorithm and the design techniques using experimental data

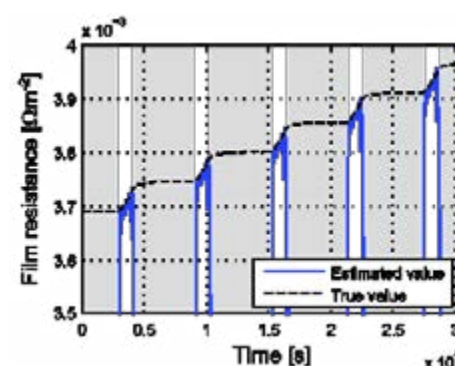


Figure 1. Battery SoH identification results. White regions correspond to constant-current charging where SEI film growth is consequential. Shaded regions represent constant-voltage charging and discharging regions where SEI film growth is negligible and hence unidentifiable from the data collected in those regions.

## Advanced Lightweight Materials and Structures

## Forming Processes for Lightweight Materials

Joint Project

U.S. Research Team Lead	China Research Team Lead
<ul style="list-style-type: none"> <li>• Jun Ni, University of Michigan</li> <li>• Glenn Daehn, The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>• Baicheng Liu, Tsinghua University</li> <li>• Xinmin Lai, Shanghai Jiao Tong University</li> </ul>
U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• University of Michigan</li> <li>• The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>• Tsinghua University</li> <li>• Shanghai Jiao Tong University</li> </ul>

*Research Objective*

This project will develop high-quality and economical bulk forming processes for lightweight materials, including aluminum and magnesium alloys, carbon-fiber composites, and high-strength steel and ultra-high-strength steel.

*Technical Approach*

- Complete a high-vacuum die casting and squeeze casting of aluminum and magnesium alloys (Tsinghua University), including porosity reduction and brittleness improvement, with close collaboration on warm forming research at the University of Michigan
- Pursue continuous compression molding of carbon-reinforced polymer composites (The Ohio State University) using inexpensive feedstock resin design
- Achieve the stamping of high-strength steel and ultra-high-strength steel (Shanghai Jiao Tong University) as well as formability

*Significant Results*

The main results of this project include the following:

- Die design and manufacturing of a crash box component of AM60B alloy under vacuum condition were conducted and numerical simulation of the mold filling of the die casting was made to optimize the die design. Die casting experiments of the crash box were conducted and castings with/without vacuum condition were provided for future evaluation on both mechanical properties and crashworthiness properties
- In order to have a good understanding on the process-structure-property of squeeze casting magnesium alloy, experiment work

was conducted, where the temperature inside the casting during the solidification under pressures up to 130 megapascals was directly measured. Further, a phase field model was developed to study the precipitation during the aging process of the casting because the casting produced under high pressure has very good integrity and can be strengthened by heat treatment (solid solution plus aging)

- Tsinghua-GM collaboration and two joint papers published in *Scripta Materialia*
  - Guomin Han, Zhiqiang Han, Alan A. Luo, Anil K. Sachdev, and Baicheng Liu. "A phase field model for simulating the precipitation of multi-variant  $\beta$ -Mg<sub>17</sub>Al<sub>12</sub> in Mg-Al based alloys." *Scripta Materialia*, Vol.68, No.9, 691-694 (2013)
  - Zhiqiang Han, Xiaoran Huang, Alan A. Luo, Anil K. Sachdev and Baicheng Liu. "A quantitative model for describing crystal nucleation in pressurized solidification during squeeze casting." *Scripta Materialia*, Vol.66, No.5, 215-218 (2012)

*Future Plan*

- Microstructure and mechanical properties analysis (Xiong) and crashworthiness analysis (Zhou) of the crash box components (with/without vacuum)

- Microstructure and mechanical property test and data analysis focusing on the correlation between the cooling curves and microstructure as well as the effect of squeeze casting process on the microstructure and mechanical properties (Han)

*Expected Outcomes*

- Experimental data of desirable windows of process parameters
- Experimentally validated simulation models of the processes
- Part design rules for higher part quality and lower production costs
- Optimized process designs
- New out-of-autoclave processes for high-strength carbon-fiber thermoplastic composites

## Advanced Lightweight Materials and Structures

## Cost Effective Lightweight Materials

Joint Project

U.S. Research Team Lead	China Research Team Lead
<ul style="list-style-type: none"> <li>• Jose M. Castro, The Ohio State University</li> <li>• Ziwei Zhao, The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>• Na Zhang, Zhengzhou University</li> </ul>
U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• The Ohio State University</li> <li>• Nano Materials Innovation</li> </ul>	<ul style="list-style-type: none"> <li>• Zhengzhou University</li> </ul>

*Research Objective*

The objective of this project is to develop cost-effective, lightweight structures for next-generation vehicle. A key barrier is the balance of processability and performance of the new composites. This project focuses on developing nano-enhanced fiber-reinforced polymeric composites (FRPCs) with adequate processability.

*Technical Approach*

- Use spray with vacuum to spray CNF-Acetone solution into glass fiber preforms to enhance their bulk properties. Then, researchers will fabricate CNF-enhanced FRPCs in the vacuum assisted resin transfer molding (VARTM) process. Adding CNFs in composites increases their mechanical performance
- Measure mechanical properties, electromagnetic interference (EMI) shielding effectiveness, and surface sand abrasion resistance to evaluate their performance
- Measure the permeability of glass fiber with/without CNFs to evaluate the processability

*Significant Results*

Experiments have been done in collaboration with Na Zhang from Zhengzhou University China.

Mechanical properties of nano-enhanced glass reinforced composites were measured. Tensile strength increased about 20%. (Figure 1)

The permeability of fiber preform with nanoparticles was measured. (Figure 2)

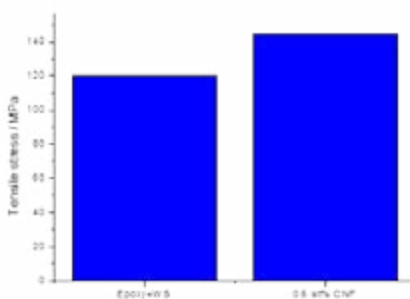


Figure 1: Tensile strength increase of glass fiber composites with/without CNFs.

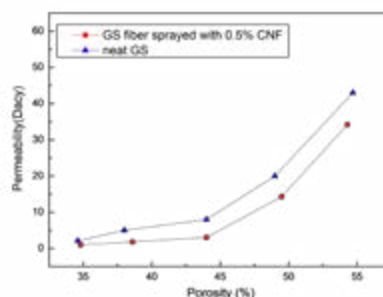


Figure 2: Permeability decreases of glass fiber with/without CNFs.

*Future Plan*

The suspending liquid will be changed to water instead of acetone to make the process environmentally friendly. Different surface modifications developed by Nano Materials Innovation will be tested for improved CNF dispersion. Researchers will also increase the amount of CNF in the surface to improve abrasion resistance as well as to form a continuous layer of CNF for improved conductivity and EMI shielding. This approach will be contrasted with using a CNF nanopaper in the surface of the composite.

To evaluate the processability of composites with a CNF layer, researchers will develop mathematical models to describe the flow. Researchers will also study the use of CNF to improve mechanical performance for parts with substructures. They will also add CNF to resin-rich regions.

*Expected Outcomes*

- Improvement in sand abrasion resistance and EMI shielding effectiveness with respect to conventional composites
- A mathematical model to describe the flow and support processability studies
- Two ANTEC-Society of Plastic Engineers (SPE) conference papers were published in collaboration of Ziwei Zhao (The Ohio State University) and Na Zhang (Zhengzhou University):
  - Z. Zhao, N. Zhang, J. L. Lee, J. M. Castro. "Manufacturability Study of Nano-enhanced Fiber Reinforced Polymeric Composites (FRPC)." ANTEC, SPE (2013)
  - N. Zhang, Z. Zhao, Y. Hioe, C. Shen, L. J. Lee, J. M. Castro. "Effect of Incorporating Nanoparticles into Fiber Reinforced Epoxy Composites." ANTEC, SPE (2013)
- Two journal papers are expected to be published based on the two conference papers

## Advanced Lightweight Materials and Structures

# Dynamic Characterization of Spot Welds for Advanced High Strength Steel

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• The Ohio State University</li> <li>• Argonne National Laboratory</li> <li>• University of Michigan</li> <li>• Sandia National Laboratories</li> <li>• Oak Ridge National Laboratory</li> </ul>	<ul style="list-style-type: none"> <li>• Tsinghua University</li> <li>• Beijing Institute of Technology</li> </ul>

## Research Objective

The project is using finite element method (FEM) crash analysis to improve prediction of spot weld failure of high-strength steels.

## Technical Approach

- Develop modeling methods of spot weld failure based on a study of welding processes and the failure mechanism of spot weld (Oak Ridge National Laboratory [ORNL])
- Conduct coupon tests of spot-welded specimens under impact loading for characterizing the failure mechanism and providing ORNL with experimental data to validate the model (Tsinghua University)

## Significant Results

The prediction of spot weld failure of advanced high-strength steel (AHSS) in FEM crash analysis is generally unsatisfactory, which greatly affects the overall accuracy of crash analysis of welded structure components. The goal of this collaborative project is to provide a modeling tool that incorporates spot weld behavior. The tool should be practical to use in vehicle crash computer-aided engineering (CAE) analysis, enabling more efficient design of AHSS structures for lightweighting while meeting crash requirements and cost effectiveness.

## Future Plans

The experimental work is ongoing.

## Expected Outcomes

- A spot weld modeling tool capable of incorporating spot weld behavior for use in vehicle crash CAE analysis
- In-depth understanding of the failure mechanism of AHSS spot weld
- Joint publication of the research results

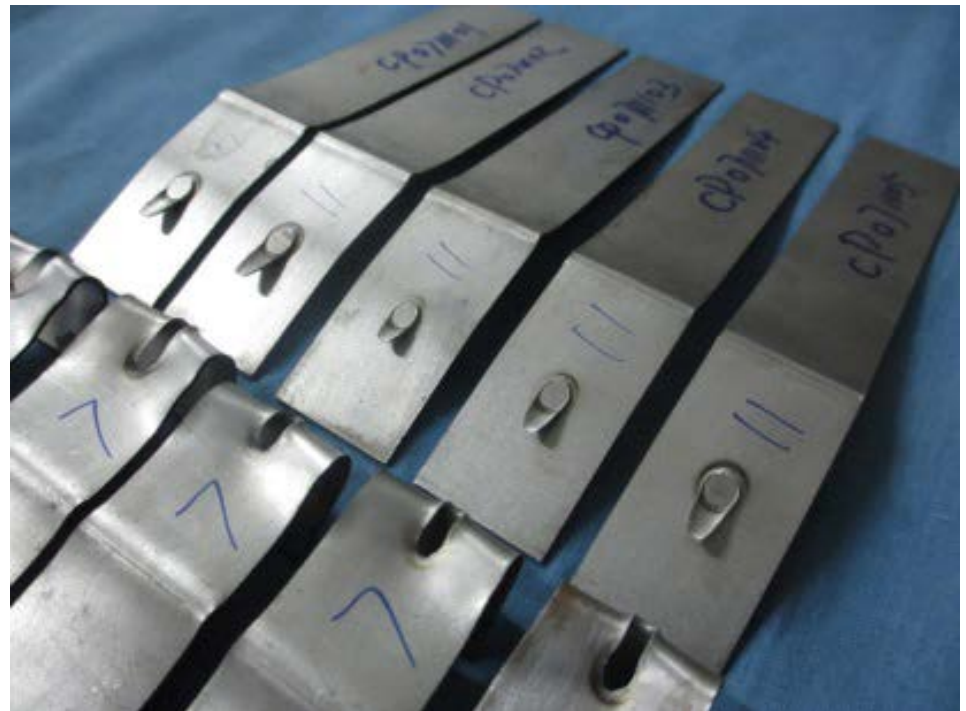


Figure 1. Post-test specimens of spot-welded coupons.

## Advanced Lightweight Materials and Structures

## High Density Battery Chemistries

Cooperative Project (U.S.)

## U.S. Research Team Lead

- Glenn S. Daehn, The Ohio State University
- Anthony Luscher, The Ohio State University
- Matthew Hansen, The Ohio State University
- David Backus, The Ohio State University
- Nolan Windholtz, The Ohio State University

## U.S. Partners

- The Ohio State University
- General Motors
- University of Michigan
- Oak Ridge National Laboratory

*Research Objective*

This project uses an integrated approach of experimentation and modeling to establish if robust and durable multi-material structures can be created by the conformal interference joining of aluminum tubes and extrusions onto aluminum or steel nodes. Such a joint morphology could help produce multi-material structures with reduced weight and improved crash resistance; stiffness; and noise, vibration, and harshness characteristics.

*Technical Approach*

- Electromagnetic forming has been used to lock favorable residual stresses into conformal interference joints. The process uses Lorentz repulsion to produce high-velocity motion of an extrusion. This can be accelerated onto a mandrel or expanded into an opening
- Instrumented experiments were combined with numerical modeling and simulation using LS-DYNA to produce a predictive design tool
- A key question was whether insulating polymeric layers could be used between the primary components to produce a system that does not suffer from any galvanic corrosion
- Initial efforts also explored the fatigue resistance of these pairs
- This project was carried out using partial support from other gifts and grants, with particular support from the Alcoa Foundation and Ohio State University Fellowships

*Significant Results*

This project established many important elements.

- Steel nodes can be attached to aluminum tubes with no reduction in the load-carrying ability. This can be superior to welding in many applications because there is no distortion or loss in strength, and almost arbitrary dissimilar metals can be joined in this way



Figure 1. Steel nodes crimped on an aluminum tube and tested in tension.

- A methodology was developed in LS-DYNA to predict the magnetic pressures required to fill varied geometries and the residual stresses that were generated during the forming process. An example is shown in Figure 2
- Simulations demonstrated that the pullout behavior could be modeled using LS-DYNA
- Experiments demonstrated that a thin (125 micrometers) polycarbonate layer could be inserted between the mandrel and the tube and could provide full galvanic isolation. This can provide excellent corrosion resistance

*Future Plan*

This area remains quite promising and is shown to be largely ready for commercial use. If and when specific geometric locations in automotive structures that will make use of these methods to join dissimilar metals are identified, focused research can be carried out to validate this for the particular joint configuration and set of materials of interest.

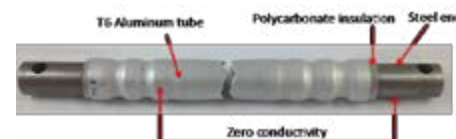


Figure 2. 6061 T-6 aluminum, 0.005" polycarbonate, and steel.



## Advanced Lightweight Materials and Structures

## Hybrid Friction Stir Welding for Dissimilar Materials

Joint Project

U.S. Research Team Lead	China Research Team Lead
<ul style="list-style-type: none"> <li>Jun Ni, University of Michigan</li> </ul>	<ul style="list-style-type: none"> <li>Xinming Lai, Shanghai Jiao Tong University</li> </ul>
U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Michigan</li> </ul>	<ul style="list-style-type: none"> <li>Shanghai Jiao Tong University</li> </ul>

*Research Objective*

The objective of this project is to develop high-quality and economical joining processes between dissimilar lightweight materials, especially for aluminum alloys and advanced high-strength steels (AHSSs). To both enhance joint quality and enlarge the process window, the project team is considering incorporating electro-plastic effect (EPE) into traditional friction stir welding (FSW).

*Technical Approach*

- Study the effectiveness of EPE through uniaxial tensile tests under high-current-density pulses on one group of AHSSs, TRansformation-Induced Plasticity (TRIP) 780/800
- Interpret observed material softening phenomenon from the perspective of martensitic phase transformation. Employ X-ray diffraction analysis to quantify phase compositions of TRIP 780/800
- Conduct a process parameter study of FSW aluminum (Al) 6061 to 304 stainless steels under different tool rotational speeds, welding speeds, tool offsets, and tool materials
- Design and realize applicable equipment for electrically assisted FSW

*Significant Results*

EPE describes the material softening phenomenon induced by current during plastic deformation. Beyond the inevitable resistance heating effect, moving electrons themselves can dynamically change the material behavior in the plastic straining range without substantial temperature increase. This effect can therefore facilitate plasticized material flow, which is one of the essential elements of FSW. In addition, a slight temperature increase restricts the expansion of the FSW heat-affected zone and increases joint strength accordingly. Although EPE has been explored on various materials, few studies have been carried out on AHSSs. In this project, the effectiveness of EPE on AHSS was first validated. One of the typical true stress-strain curves under four current pulses with a current density of 29.7 amperes per square millimeter (A/mm<sup>2</sup>) is shown in Figure 1.

An empirical exponential model relating true stress to true strain was adopted to fit the material behavior under pulses. Fitted curves

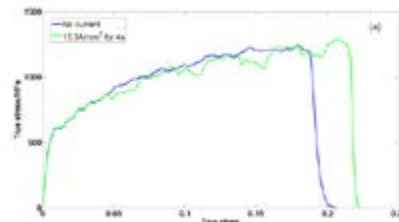


Figure 1. True stress-strain curve for TRIP 780/800 under current pulses.

are shown in Figure 2, which shows that 7.4 A/mm<sup>2</sup> is the threshold current density for EPE on TRIP 780/800.

Because the mechanical behavior of TRIP 780/800 depends greatly on the martensitic phase transformation during plastic straining,

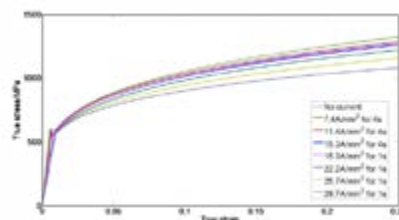


Figure 2. Fitted true stress-strain curves on TRIP 780/800.

the research team carried out X-ray diffraction analysis to quantify the volume fraction of retained austenite after tensile testing. The results are shown in Figure 3, which illustrates that the applied current retarded the phase transformation process.

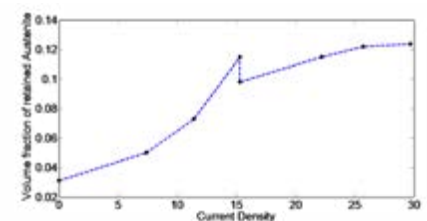


Figure 3. Volume fraction of retained austenite with regard to current density.

Tensile tests with high-current-density pulses were also performed on Al 6061. The results (shown in Figure 4) indicate that under the same current density of 20 A/mm<sup>2</sup>, the drop in flow stress for Al 6061 is negligible compared with that for TRIP 780/800.

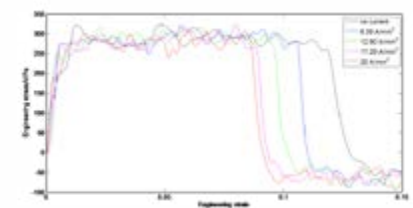


Figure 4. Electrically assisted tensile test for Al6061.

Preliminary experiments on FSW of Al 6061 with 304 stainless steels were performed. Researchers applied three different rotational speeds (600, 1200, and 1800 rpm) and welding speeds (30, 60 and 90 mm/min). Both the axial and traverse welding forces were recorded during the process; Figure 5 shows a typical curve and Figure 6 shows a welded sample. Results show that if the rotational-speed-to-traverse-speed ratio is too high, tunnel defects can form. On the other hand, if the ratio is too low, surface grooves can develop. Therefore, the optimum combination of rotational speed and traverse speed must be identified. As for the welding force, higher rotational speed can greatly reduce the axial force during the plunge stage, but the effects of higher rotation speed during the traverse stage were not obvious.

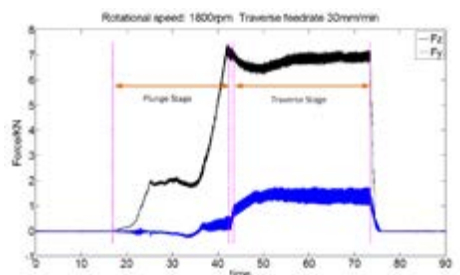


Figure 5. Typical welding force during FSW.

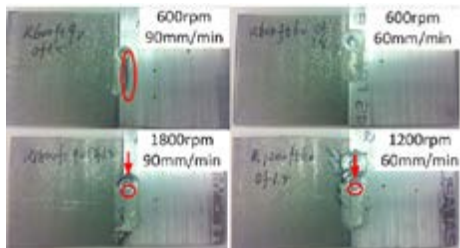


Figure 6. A welded specimen under different welding parameters.

### Future Plans

The project team will use more refractory materials, such as tungsten carbide or even polycrystalline cubic boron nitride, as the FSW tool material, which will alleviate severe tool wear from shifting the tool more toward the steel side. Researchers will use both mechanical tests and microstructure analysis to examine joint quality. They will also establish a finite element model to study the welding mechanism, which will help predict process force and temperature. Researchers will also complete the experimental arrangement for electrically assisted FSW. They will join the two materials under study, Al 6061 and TRIP 780/800, and after measuring force and temperature and evaluating joint quality, the research team will compare the results with data from a traditional FSW process.

### Expected Outcomes

- Improved quality of the joint between Al 6061 and TRIP 780/800
- Reduced mechanical force during FSW

## Advanced Lightweight Materials and Structures

# Multi-Material Lightweight Body Subsystem and Vehicle Optimization

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Michigan</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> <li>Shanghai Jiao Tong University</li> <li>Tongji University</li> </ul>

## Research Objective

The project is developing a methodology for economically integrating components made of lightweight materials in vehicle body structure with maximum weight reduction benefit. The materials under consideration are aluminum, magnesium, high-strength steels (HSSs) and ultra-high-strength steels (UHSSs), and composites.

## Technical Approach

- Determine deformation control and failure prevention strategy; exploration of innovative load paths, crash modes, and component layouts (Tsinghua University)
- Predict assembly dimensional variations: modeling of lightweight material process variations (Shanghai Jiao Tong University)
- Establish evaluation criteria for ease of manufacture and assembly: modeling of constraints for lightweight material processes (forming and joining) on part and joint geometry (University of Michigan)
- Enable multi-material optimization of vehicle body (sub)systems: a simplified body-in-white of a mini electric vehicle (EV) and an extended A-pillar of a midsize vehicle (all partners)

## Significant Results

To avoid duplicating previous work, the project team first closely studied final reports of the two recently completed vehicle lightweighting projects conducted by the U.S. Environmental Protection Agency and the National Highway Transportation Safety Administration. The project team concluded that both projects lacked realistic modeling of multi-material joints and of geometric constraints imposed by forming and joining processes of lightweight materials.

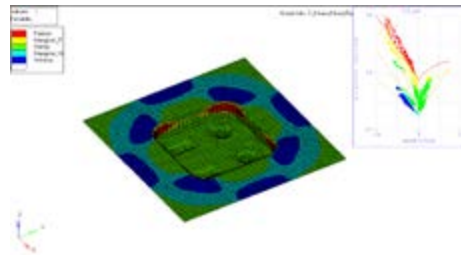


Figure 1. Simulation result of sheet-stamping process of one of approximately 1,000 sample parts with typical features.

To address one of these gaps, researchers first did data mining of process simulation results of lightweight parts and joints. Based on the results, the team developed a methodology for generating design for manufacturing (DFM) and design for assembly (DFA) guidelines. The Shanghai Jiao Tong University team members are applying the methodology to the HSS/UHSS stamping process (see Figure 1).

The project also evaluated the safety of the designed mini-EV body structure (Figure 2, top). Researchers used the finite element method (FEM) to study the effects of alternative load paths and battery layouts on crashworthiness (Figure 2, bottom). The team is also using computational fluid dynamics analysis on the same body model to optimize its aerodynamic performance.

To predict dimensional variation in multi-material assemblies, researchers used FEM to study the effects of variations in fixture and welding locations (Figure 3, top) and of variations in temperature (Figure 3, bottom).



Figure 2. Parameterized computer-aided design (top) and computer-aided engineering (bottom) models of a mini-EV.

## Future Plans

In 2013, the team plans to (1) study the crashworthiness and impact protection of mini-EV batteries, (2) conduct optimization studies of the weld locations in the presence of fixture and temperature variations to minimize dimensional variations in multi-material assemblies, (3) apply the developed DFM/DFA guideline generation method to forming and joining processes investigated in other projects with related scope, 4) conduct multi-material optimization of the mini-EV, and 5) develop a parameterized CAE model of an extended A-pillar of a midsize vehicle.

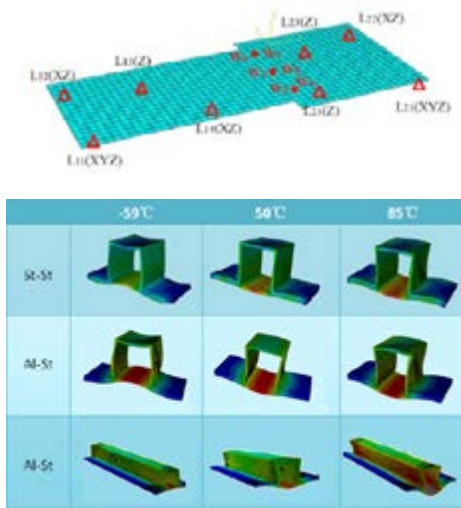


Figure 3: Finite element simulation of variation in multi-material assemblies due to fixture and welding (top) and due to environmental temperature (bottom).

### *Expected Outcomes*

- Architecture and material selection strategy for mini-EV crash safety, including the protection of batteries
- Guidelines to reduce dimensional variations of multi-material assemblies due to the variations in fixture, joints, and environmental temperature
- Optimization method for multi-material vehicle body subsystems, incorporating manufacturability and ease of assembly criteria

## Vehicle Grid Integration

# System Architecture and Interaction Mechanism of ITS Based V2G

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> </ul>

## Research Objective

The project is studying the mechanism of the interaction between the power system and the transport system when electric vehicles (EVs) are in operation. The research aims to employ an integrated communication platform and optimization strategy to sustain the electricity system's and transportation system's high-efficiency performance.

## Technical Approach

- Investigate the mechanism and influence of EVs in operation on the power system and the transport system, and recommend a route-planning strategy based on overall system optimality
- Characterize EV charging loads based on statistical data from the 2009 National Household Travel Survey and envisioned real-time Intelligent Transportation System (ITS) data; develop an advanced method for evaluating EV charging impacts on the distribution grid
- Study the economy of coordinated EV charging with large-scale wind farms integrated into the transmission grid
- An optimization method has been developed for managing EV charging by using an aggregator to track the purchased power profiles in the distribution network

## Significant Results

Many European and U.S. research organizations have programs that survey the interaction between the electricity system and the transport system. This research project has studied many of these related programs, including ELVIRE, eCo-FEV, EcoGem, EFUTRUE, EMERALD, and Mobility 2.0. Based on the team's collective understanding of the existing research programs, the project has expanded the concept of the ITS-based vehicle-to-grid system. The collaboration has established four work packages: driving safety, energy efficiency, driving confidence, and comfort.

With a large number of EVs in operation, researchers studied the optimal charging station location strategy, aiming to coordinate the electricity system and the transport system.

Based on the nearest charging station to EVs (located in accordance with recommended strategy), researchers simulated adverse impacts on the road network and electricity system.

Simulation results clarify that the currently recommended strategy for determining the nearest charging station location will burden both the electrical and transport systems.

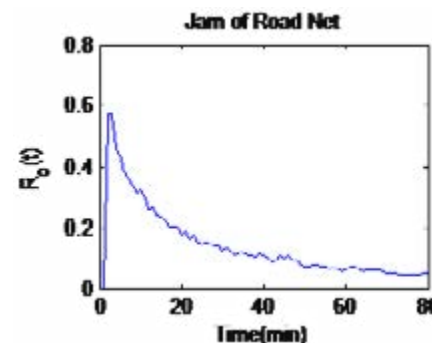


Figure 1. Road work congestion ratio with the time variation.

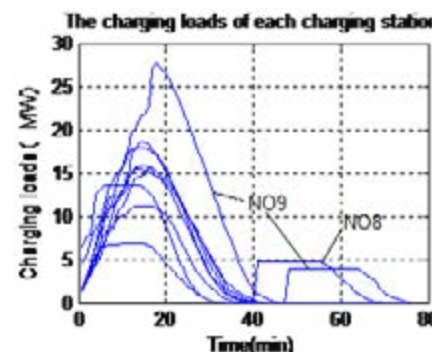


Figure 2. The charging loads of each charging station.

The project team also studied characteristics of EV charging loads, recognizing and analyzing the main influencing factors. The results are shown in Figure 3.

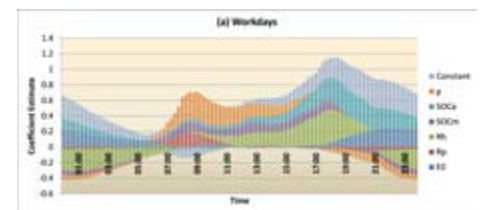


Figure 3. The characteristics of an EV charging load.

The team also studied a Global Power Flow (including transmission and distribution system)-based EV charging evaluation method. The traditional evaluation method often provides overly optimistic results; the method under study addresses this flaw and therefore might be a more useful tool for security evaluations of power systems with large-scale EV integration.

Research also investigated the economics of wind-EV coordination. The team concluded that great win-win benefits can be achieved for both the power system and EV owners. Not only are there significant reductions in total system operation costs, wind curtailment, and emissions, but also EV owners' charging fees decrease.

Finally, the project team studied a rigorous distribution optimization method for managing EVs charging in an aggregator. An aggregator has many EVs. The team aims to manage those EVs so that the total power curve of the aggregator would track the scheduled one. Researchers proved mathematically that the solution is optimal. Numerical tests indicate that the method is also scalable for large numbers of EVs.

## Future Plans

The project plans to develop a method to estimate the remaining range for an EV based on traffic information. The team will continue efforts to improve the charging station recommendation strategy with the aim of coordinating the electricity system and transport system. Eco-route planning is also a project objective; the planning will consider battery characteristics and real-time information. Finally, researchers will continue to investigate wind-EV coordination, with more security constraints and unit commitment as two points to consider.



### *Expected Outcomes*

- A valid algorithm for the remaining range estimation and eco-route planning
- A charging station recommendation strategy with overall performance coordination between the electricity grid and transportation system
- A mechanism for EV charging load distribution
- A mechanism for wind-EV coordination under complex situations

## Vehicle Grid Integration

# EV Intelligent Control Based on Vehicle-Grid-Infrastructure Interaction

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>The Ohio State University</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> </ul>

## Research Objective

As the number of EVs in operation increases, there is a parallel need to coordinate the Intelligent Transportation System (ITS), the smart grid, and electric vehicles (EVs). Such coordination would enhance overall EV safety, fuel efficiency, and ride comfort. This project includes EV path planning and driver assistance control based on vehicle-grid-road safety and efficiency coordination. To improve driving comfort, the project is developing an automatic charging station guidance system based on vehicle charging station communication.

## Technical Approach

- Develop an integrated EV communication platform with road infrastructure, ITS center, power grid, and other EVs
- Effect EV eco-route planning while considering real-time traffic and battery characteristics
- Produce EV integrated chassis control (ICC), incorporating longitudinal/lateral safety and fuel economy
- Develop autonomous guidance for EVs in the charging station

## Significant Results

The project team obtained real-time and accurate estimations of longitudinal velocity and vehicle sideslip angles. To achieve these results, researchers combined signals from global positioning systems and inertial navigation systems, integrating kinematic and dynamic estimation methods.

Researchers also developed optimum tire force distribution based on the performance index of tire workload and tire energy dissipation. The project team proposed a dynamic target regulation method to obtain the desired longitudinal and lateral tire force based on driving conditions.

The team also used an inverse tire model to transform the desired longitudinal and lateral tire force to tire slip ratio and sideslip angle. The tire slip ratio and sideslip angle are controlled by a sliding mode controller and a combined feed forward/feedback controller, respectively.

The project team proposed a path tracking control algorithm for driving an EV automatically inside of a smart charging station from the entrance to the charger. The team implemented a bicycle vehicle model when developing a first-order steering shaft model, magic formula for tires, and Ackerman steering model. To reduce the lateral error between the desired track and real track, which the vehicle would follow, the researchers are controlling the look-ahead distance parameter of the control

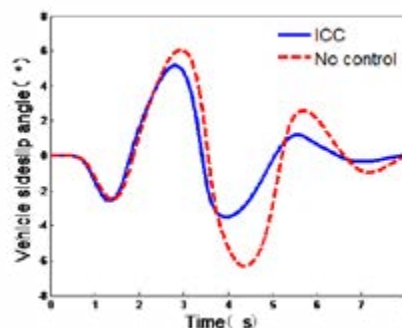


Figure 1. Comparison of simulation results showing the sideslip angle for a smaller vehicle without control versus a vehicle with ICC.

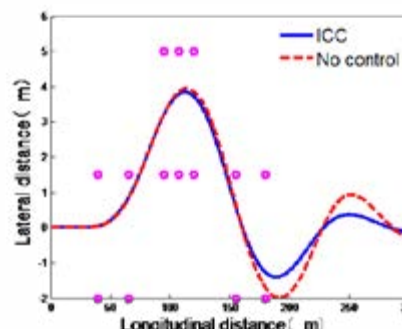


Figure 2. Simulation results showing improved stability for a vehicle with ICC.

algorithm, which depends on the vehicle speed and path curvature of the track. Finally, to plan EV motion that would bring the car to the charger, researchers chose a fuzzy logic path tracking strategy marked by clarity of code, simple structure, and low computational cost.

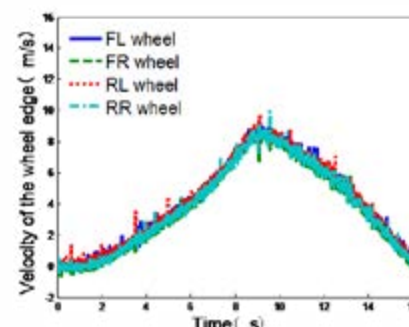


Figure 3. Test results showing that all the wheels of a vehicle with ICC are controlled well with no slip.

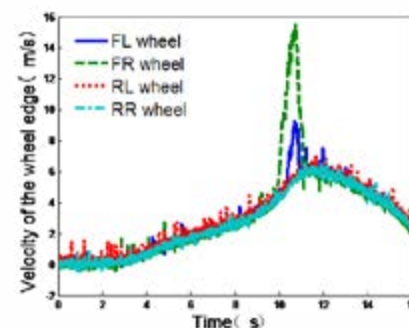


Figure 4. Test results showing slip in front left and front right (FL and FR) wheels of a vehicle with no control.

## Future Plans

Next steps include running vehicle experiments to verify the control algorithm for autonomous EV guidance in a charging station. Researchers will also continue work on the EV eco-route planning algorithm based on traffic information and predictive energy consumption, as well as an integrated EV control strategy that considers vehicle economy performance.

## Expected Outcomes

- Valid control algorithm for autonomous EV guidance in a charging station
- An ICC control strategy that enhances vehicle economy performance

## Vehicle Grid Integration

# Vehicle-Grid System Modeling for Technology Deployment

Joint Project

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U.S. Partners	China Partners
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## Research Objective

The objective of this project is to assess the impact on the electric grid of a large-scale deployment of plug-in electric vehicles (PEVs). The project team will also develop a technology roadmap and policy recommendations for accelerating PEV deployment in the United States and China.

## Technical Approach

- Develop a comprehensive suite of PEV technology adoption, PEV driving, PEV charging, and power system unit commitment and economic dispatch models
- Use these models in an integrated fashion to examine how PEV adoption and use can affect power system economics, operations, reliability, and capacity planning
- Capture demographic, socioeconomic, and spatial and social network impacts and associated clustering of PEVs and charging loads using the PEV technology adoption model
- Use simulation techniques to model PEV driving and grid-connection behavior
- Combine simulated PEV driving and charging demand profiles with power system operation models to study interactions between PEVs and the power system, the use of control, and other techniques to mitigate adverse effects
- Use results of these modeling efforts to develop technology and policy roadmaps that are specially tailored to vehicle and power system markets in the United States and China

## Significant Results

Work on this project is proceeding in three main areas. First, the project has developed a comprehensive optimization/simulation model to locate public PEV charging infrastructure within a metropolitan area. This provides useful decision-making tools for public entities and private enterprises planning PEV charging station deployments. This model accounts for actual driving behavior and its inherent randomness and determines where best to locate charging stations with fixed resource constraints. A case study, based on the central Ohio region, demonstrates the flexibility of this framework to capture different optimization criteria. The U.S. and China teams are collaborating to expand this work to endogenously capture PEV destination decision making based on charging station availability.

Second, researchers are using actual vehicle adoption data to develop and calibrate spatial econometric models of PEV adoption. Given the relatively small penetration of pure PEVs, other advanced-technology vehicles (e.g., turbodiesels) and hybrid electric vehicles (HEVs) are being used as proxies for PEV adoption. Preliminary testing, using county-level HEV adoption data for the state of Ohio, shows strong spatial correlation in adoption patterns. The researchers will collect census-block-level vehicle adoption data from the Ohio Bureau of Motor Vehicles, then use these data to further refine the model. Modeling and predicting the location of PEV owners is important for utility distribution infrastructure planning, given the new loads that these vehicles impose on distribution feeders and transformers. These models can also be useful to firms marketing PEVs and other advanced vehicle technologies.

Third, the project team is exploring the use of price-based schemes to control PEV charging in a decentralized manner. The purpose of these control schemes is to coordinate PEV charging with power system operations. PEV economics can be substantively improved if PEVs charge



Figure 1. PEV charging infrastructure location optimization model results for central Ohio.

at the “correct” time, when excess generating capacity is available. Moreover, PEVs can also provide an added source of demand flexibility to aid the integration of variable renewable resources, such as wind and solar. This work focuses on using iterative price-update schemes to efficiently guide PEV owners and load aggregators to charge vehicles at times that are mutually beneficial to the power system and PEV owners. These control schemes will also be refined to ensure algorithmic efficiency (i.e., PEVs converge to a desirable charging profile with minimal communication overhead required between vehicle owners and the electric utility).

## Future Plans

Future work will focus on developing PEV swarm models to fully simulate the distribution- and bulk-power-system-level impacts of large PEV fleets. These models will highlight benefits and potential risks of large-scale PEV adoption. Based on these findings, technology and policy recommendations to mitigate any adverse impacts will be made. Policy recommendations will also be made for deployment and development of PEV technologies and related infrastructures in the United States and China.

### *Expected Outcomes*

- A flexible model to optimize the location of public charging infrastructure in different regions and with different optimization criteria and resource constraints
- PEV adoption models that capture the effects of demographics, socioeconomics, and social and geographic spatial networks
- Models and tools to analyze PEV impacts on the electric grid, at both the local distribution and bulk power system levels
- Policy recommendations for cohesive development and deployment of PEV technologies and related infrastructure in the United States and China
- Optimized control strategies for vehicle-electric grid interactions, including centralized and market-based approaches

## Vehicle Grid Integration

## Control Strategies for Vehicle-Grid Integration

Joint Project

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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>University of Michigan</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> </ul>

*Research Objective*

The project seeks to develop control strategies that mitigate distribution-level issues associated with high penetration of plug-in electric vehicles (PEVs) and that allow PEVs to provide operational services to the wider grid. A range of operational services are being considered, including peak reduction, regulation, spinning reserve, and the use of load to track variability in renewable generation.

*Technical Approach*

- Establish distributed control strategies for coordinated charging of large populations of PEVs
- Construct a wireless test bed to quantify the characteristics and effectiveness of distributed control strategies for PEV charging
- Study the response of PEV chargers to grid voltage abnormalities

*Significant Results*

Results include the development of distributed control algorithms for regulating the charging of PEVs on power system distribution networks. Investigations have confirmed that distributed control provides a practical approach to scheduling PEV charging for residential customers. This knowledge is useful to both utilities and car manufacturers in designing systems that use the inherent storage capability of PEV batteries to increase power system reliability. The techniques under development enable PEVs to optimally use non-dispatchable renewable resources such as wind and solar power.

A distributed control algorithm has been developed for coordinating PEV charging so that distribution transformers do not become overloaded. This algorithm quantifies the heating effect of the current drawn by the background load together with the PEV charging load and establishes a pseudo-price signal that is communicated to the PEVs. Using that information, PEVs establish a charging strategy that ensures the transformer temperature does not rise to an unacceptable level.

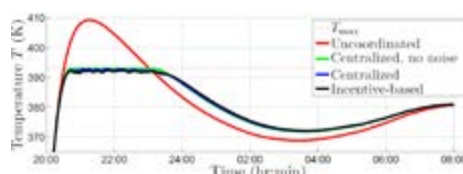


Figure 1. Transformer temperature: uncoordinated and controlled PEV charging.

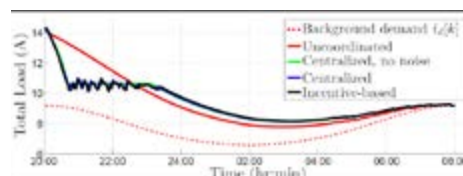


Figure 2. Total load supplied by the transformer: uncoordinated and controlled PEV charging.

The project team has also developed a test bed to analyze the feasibility and response of proposed charging algorithms in the presence of realistic physical constraints including communication time delays, microprocessor memory limitations, and battery charging dynamics. The researchers determined that relatively simple strategies, such as an additive-increase-multiplicative-decrease algorithm, can achieve good quality load response with minimum communications infrastructure. It is also feasible for more computationally intensive techniques such as model predictive control to regulate PEV charging at near-optimal levels, but at the expense of greater memory and communications requirements.

The project has explored the development of iterative schemes in which each PEV minimizes its own charging cost, while the collective behavior of the PEV population converges to a Nash equilibrium that optimally fills the overnight demand valley. Extensions include the introduction of a terminal cost associated with not fully charging the battery, and methods for incorporating heterogeneity in the PEV population.

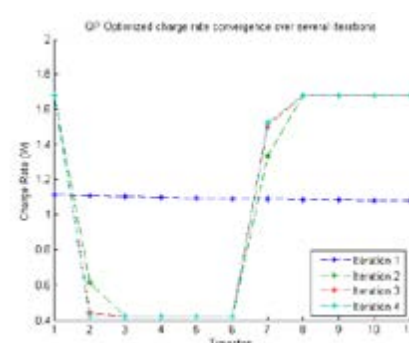


Figure 3. Charging rates quickly converge to an optimal global solution.

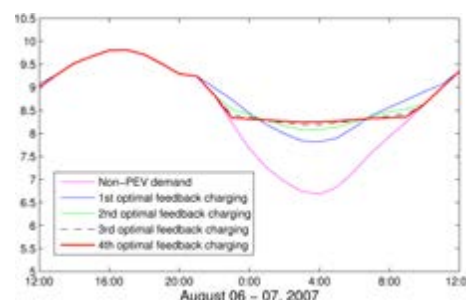


Figure 4. Iterative convergence of decentralized charging control.

Researchers have also developed hysteresis-based charging control strategies to coordinate the aggregate demand of a population of PEVs. Such strategies enable the total PEV demand to track variations in the output of renewable generation.

PEV charging equipment is likely to trip if the grid voltage sags below 80% of nominal. If such a grid disturbance affects a large number of PEVs, the resulting loss of load could lead to unacceptably high voltages once the initiating event has been cleared. The most effective way to prevent such problems is to reformulate standards to enforce low-voltage ride-through for PEV chargers.



### *Future Plans*

Test-bed development will include upgrading the computational capability of battery chargers to reduce algorithm analysis time. Robustness of the control algorithms will be explored through implementation of various forms of background demand disturbances.

Hysteresis-based control algorithms will undergo further development to achieve improved tracking performance. Nonlinearities associated with such control schemes will be explored.

Nash-based valley-filling control strategies will be extended to consider the effects of transmission line congestion.

### *Expected Outcomes*

- Distribution-level control of PEV charging
- Control strategies for grid operational services
- Coordination of PEV charging with renewable generation
- Decentralized control strategies for PEV charging
- An understanding of the impact of non-ideal communications networks and computational limitations on the coordination of PEV charging loads

## Energy Systems Analysis, Technology Roadmaps, and Policy

# Set CV Technology Energy Efficiency and GHG Targets and Evaluate Life Cycle Performance

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>• Argonne National Laboratory</li> <li>• University of Michigan</li> <li>• Ford Motor Company</li> <li>• Delphi</li> </ul>	<ul style="list-style-type: none"> <li>• Tsinghua University</li> </ul>

## Research Objective

The objective of this project is to define energy efficiency and greenhouse gas (GHG) targets for clean vehicle (CV) technologies and systems as well as evaluate their performance from a life cycle perspective. Different combinations of CV technologies will be evaluated from a life cycle perspective such that GHGs are minimized while vehicle performance is maintained.

## Technical Approach

- Develop life cycle models that encompass both the vehicle life cycle (materials production, manufacturing, operation, and end-of-life management) and the total fuel cycles (upstream and combustion) based on vehicle simulation
- Develop a vehicle model that accounts for functional equivalence such that proposed vehicle designs for conventional and electrified vehicles are comparable to each other in terms of acceleration and towing capabilities, cargo volume, and size
- Apply target cascading to identify best combinations of vehicle technologies that minimize GHG emissions subject to constraints of cost, performance, and other consumer attributes

## Significant Results

The project team developed a method to impose realistic limits on engine models (e.g., engine knock and flammability limits) to assess the ideal versus realistic potential of baseline and high-efficiency engines to increase vehicle efficiency. Specifically, knock and flammability limits are assessed using a combination of conceptual models based on theory and experimental results. Knock is assessed by comparing residence time to ignition delay time. Flammability limits are determined by evaluating the impact of strain on the flame using the Karlovitz number, the ratio of laminar to turbulent parameters, and the Leeds

Combustion Diagram. High-efficiency engines included downsized/boosted gasoline and ethanol engines, while the baseline model is a naturally aspirated gasoline engine. Models are implemented in GT Power and are a key aspect in further vehicle technology studies.

Researchers also developed a method for defining comparable vehicles based on functional equivalence. Factors influencing

functional equivalence include vehicle class, seating capacity, plan view area, front track width, cargo volume, acceleration, and gradeability.

The project team also analyzed detailed teardown data from 25 internal combustion vehicles (ICVs), 2 hybrid electric vehicles (HEVs), 2 plug-in hybrid electric vehicles (PHEVs), and 1 battery electric vehicle to develop a linear regression that is used to determine vehicle mass based on front track width and powertrain mass. Regression has an  $R^2$  of 0.77.

A regression analysis model was applied to determine initial vehicle designs for proposed ICVs, HEVs, and PHEVs that are functionally equivalent.

Researchers used vehicle simulation over U.S. Environmental Protection Agency (EPA) drive cycles, acceleration, and gradeability tests to identify appropriate engine sizes for ICVs and HEVs and motor and battery size for HEVs. Initial simulation results are consistent with expectations and current ICVs and HEVs.

Researchers identified subsystems within vehicles that could reasonably be lightweighted using aluminum based on material indices (closures, bumpers, and fenders). Material indices are based on force balance equations and account for both geometric constraints and structural requirements. Substitution ratios were used to replace steel with aluminum, resulting in the total vehicle mass that could be lightweighted with aluminum.

Using initial vehicle design, lightweight materials were incorporated and secondary mass reductions were determined based on mass influence coefficients. Then engine power was decreased as a result of the reduced mass, which in turn allowed for reduced engine power; the process of mass reduction iterated until a final down-sized vehicle was identified.

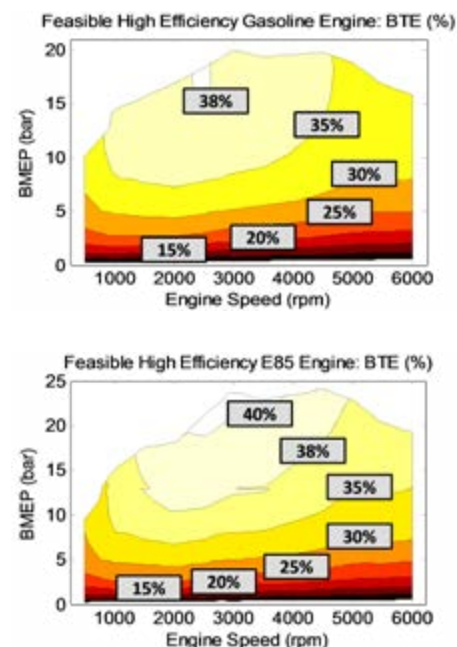
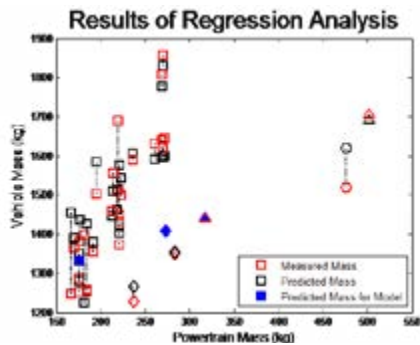
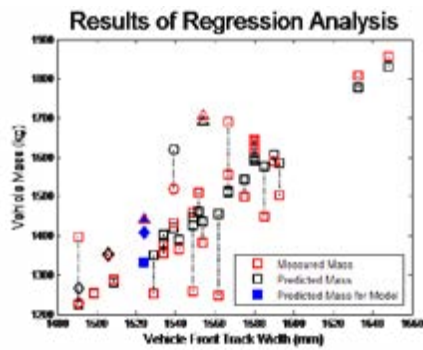


Figure 1. Brake thermal efficiency of high-efficiency gasoline and ethanol (E85) engines.



Figures 2 and 3. Results of regression analysis showing vehicle mass compared to powertrain mass and front track width.

### Future Plans

The project team will determine HEV powertrain component sizes based on a method of sizing the engine for gradeability and the motor for acceleration. Team members will use the current method to determine baseline and lightweight PHEV-40 characteristics, ensuring that the battery size meets the energy requirements to travel 40 miles in electric mode on the EPA Urban Dynamometer Driving Schedule drive cycle. Finally, researchers will determine life cycle results for baseline and lightweight vehicles.

### Expected Outcomes

- Technology performance targets that are consistent with reducing gasoline consumption (to enhance energy security and meet carbon reduction strategies) based on atmospheric carbon dioxide stabilization studies
- Life cycle models for key CV and fuel technologies (developed in other thrusts)
- An analysis of a combination of CV and fuel technologies to evaluate optimal life cycle performance
- Life cycle models of CV fuel systems for diverse driving and fueling technologies

## Energy Systems Analysis, Technology Roadmaps, and Policy

## Fuel Mix Strategies and Constraints

Cooperative Project (U.S.)

## U.S. Research Team Lead

- Dawn Manley, Sandia National Laboratories
- Ming Xu, University of Michigan

## U.S. Partners

- Sandia National Laboratories
- University of Michigan

*Research Objective*

The objective of this project is to assess the feasibility of alternative vehicle fueling, including biofuels and electricity, for meeting significant penetration of clean vehicles (CVs). This project will highlight critical resource availability and infrastructure constraints for both biofuels and electricity generation. This project will be complemented by activities that will address grid control and resilience in Thrust 6.

*Technical Approach*

- Conduct a national assessment to understand resource constraints and competition with demands from other sectors (agriculture, urban, industrial activities, etc.)
- Complete a regional analysis to develop optimized strategies to maximize the reduction of greenhouse gas (GHG) emissions and fossil fuel use, given the resource constraints
- Conduct an assessment of the feasibility and opportunities for large-scale penetration of CV and fuel technologies
- Apply the modeling framework to China

*Significant Results*

At the national level, based on existing policies, transitioning the current gasoline-based transportation into one with CVs will increase national annual water consumption by 1,950–2,810 billion gallons of water, or 1.5%–2.2%, depending on the market penetration of electric vehicles (Figure 1).

At the regional level, variances of water efficiency in producing different fuels are significant. Using an optimization approach to further evaluate impacts on regional water stress from a fully implemented CV system, we were able to identify potential roles (fuel producer or consumer) states may play in a real-world CV development scenario (Figure 2). This analysis has been submitted to *Applied Energy*.

To complement the assessment of water utilization, researchers assessed the feasibility of the U.S. light-duty vehicle (LDV) park to

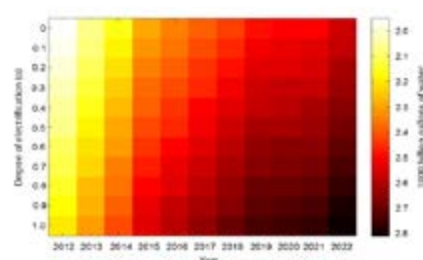


Figure 1. Projected additional water consumption due to CV deployment. Degree of electrification refers to the percentage of remained travel demand (after applying biofuels mandated by RFS2) that is fulfilled by electric vehicles (the rest by gasoline).



Figure 2. Optimized state-level water consumption and water flows embodied in interstate trade of alternative fuels. Size and color of circles indicate the amount of water consumption related to producing designated fuels, including fuels consumed within the states and those transported to other states. Lines go clockwise from states producing to states consuming designated fuels. Line color indicates the amount of water embodied in interstate trade of fuels.

consume biofuels prescribed by the modified Renewable Fuel Standard (RFS2). RFS2 prescribes the annual volume of biofuels to be used in the transportation sector through 2022 (Figure 3).

Sensitivity analyses indicate that the fuel price differential between gasoline and ethanol blendstocks, such as E85, is the principal

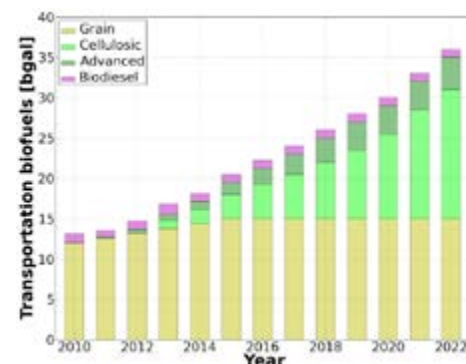


Figure 3. The Renewable Fuel Standard biofuels mandate by year. Figure from Schnepf and Yacobucci, *Renewable Fuel Standard (RFS): Overview and Issues*. Congressional Research Service (2012).

factor in LDV biofuel consumption (Figure 4). The number of flex fuel vehicles and biofuel refueling stations will grow given a favorable price differential.

However, when considering the broader goals of reducing fossil fuel consumption and GHG emissions in the context of other clean fuel

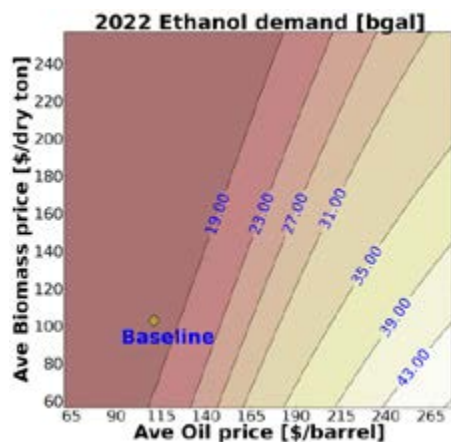


Figure 4. RFS2 can be satisfied at extreme values for oil and biomass, which make gasoline very expensive and biofuels very inexpensive. Contours represent 2022 ethanol demand in billions of gallons.

and vehicle technologies, including vehicle electrification, natural gas, and improvements in conventional vehicle powertrain efficiency, researchers have observed dynamics that illustrate competition between various CV and fuel alternatives. This analysis has been submitted to *Energy Policy* (2013).

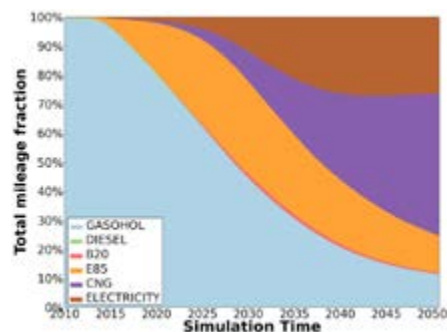


Figure 5. Mileage fraction of various fuels if commodity prices that lead to RFS2 compliance persisted through 2050. Powertrains that do not rely on gasoline would thrive.

### Future Plan

- Investigate impacts to land use intensity due to CV development
- Apply the framework on water implication to CVs in China
- Correlate water consumption analysis with analyses for CV and fuel penetration

### Expected Outcomes

- Feasibility assessments of large-scale clean fuel and vehicle technology penetration in the context of national policy goals
- Evaluation of constraints posed by critical infrastructure systems and natural resources to meet CV targets in both the United States and China



## Energy Systems Analysis, Technology Roadmaps, and Policy

# Fuel Economy and GHG Standards and Labels for PEVs from a Life Cycle Perspective

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"> <li>Argonne National Laboratory</li> <li>U.S. Environmental Protection Agency</li> </ul>	<ul style="list-style-type: none"> <li>Tsinghua University</li> <li>China Automotive Technology Research Center</li> </ul>

## Research Objective

This project is evaluating proposed fuel economy labels and greenhouse gas (GHG) standards from a life cycle perspective. The project is also evaluating and providing recommendations for alternative fuel economy and GHG assessment methods, standards, and consumer labels. Project objectives also include recommended standards based on an examination of the relationship between the U.S. Environmental Protection Agency (EPA) fuel economy metric, used for labeling, and life cycle GHG emissions for electrified vehicles. The project will quantify variations in vehicle life cycle GHG emissions due to differences in vehicle production, driving patterns, and regional electric grids. The research team will also design optimal parameters for plug-in electric vehicles (PEVs) based on the urban travel mode (e.g., vehicle miles traveled and duty cycle, among others).

## Technical Approach

- Develop a framework to explore the effectiveness of alternative assessment methods, regulatory instruments, and labeling formats to accurately represent vehicle energy and environmental performance from a life cycle perspective
- Evaluate current labels and standards from a life cycle perspective
- Evaluate long-term impacts of standards, and evaluate implications of vehicle life cycle performance compared to known targets of GHG reduction

## Significant Results

Researchers evaluated current internal combustion vehicles and hybrid electric vehicles to establish life cycle GHG correlation to fuel economy for the United States. PEV life cycle GHG emissions were compared for varying ratios of electric miles driven to total miles driven (utility factor) and varying electric grids with current EPA labels.

The major finding from the first phase of this research was that, in contrast to conventional vehicles, electric vehicles (both plug-in hybrid and all electric) do not have a direct correlation between life cycle performance and the fuel economy metric. The fuel economy metric was a useful proxy for the life cycle performance of conventional vehicles, thanks to the uniformity of gasoline emissions. Electricity GHG emissions vary widely between regional electrical grids, causing the variance for subsequent life cycle vehicle GHGs to be large as well.

Figure 1 shows the differences in life cycle GHG emissions for a plug-in hybrid electric (PHEV) with a 40-mile all-electric range based on charging in various electric grids, including the average grid in China. The figure demonstrates that in certain regions of the United States, and for the Chinese grid, the plug-in vehicle is actually responsible for more GHG emissions in electric mode than in gasoline mode.

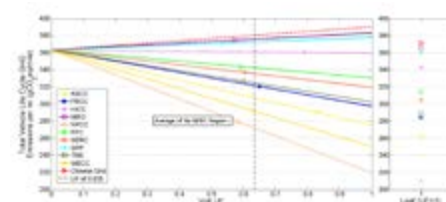


Figure 1. Differences in PHEV life cycle GHG emissions based on charging location and utility factor.

The difference between the GHG emissions reported on the PEV EPA label and the life cycle emissions is significant. The researchers recommended to the EPA that these be accounted for in the 2017–2025 Corporate Average Fuel Economy (CAFE) standards and that such information should be incorporated into EPA labels.

In the second phase of the research, the team evaluated the EPA's PEV GHG emissions accounting methodology. The current methodology, used in the EPA GHG standard for light-duty vehicles, uses projected regional hybrid vehicle sales to predict future sales of PEVs. This is compared to an approach in which associated PEV GHG emissions are calculated for the region and in the year in which the vehicles are actually sold. Findings suggest that the EPA's simplification of the market will not contribute greatly to a misallocation of GHG emissions. The EPA method greatly simplifies the accounting process.

Figure 2 shows the average U.S. electricity GHG emission factor for two different U.S. Energy Information Administration scenarios—a baseline and a carbon tax. The green bars represent the emission factor used by the EPA in its 2017–2025 standards. The blue bars represent the average electric emission factor, and the yellow bars represent the electricity GHG emission factor weighted by the PEV electricity use in different U.S. Census regions and divisions. A sales sensitivity, shown by the error bars, shows that even a tripling of sales in any one Census area from the initial sales allocation would not have a large effect on the weighted emission factor.

Another deliverable from this project is a shared thrust-area-wide wiki that allows researchers to share resources and knowledge related to data and modeling techniques. The wiki information is shared with Chinese and industrial partners.

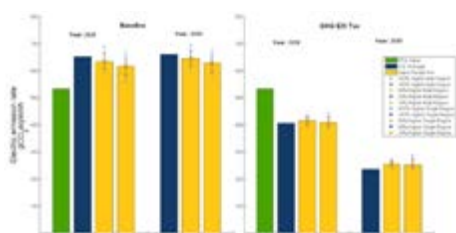


Figure 2. Study suggests that regional variation has little impact on GHG emissions. Further, long-term reductions in GHGs will likely be minimal except in a monetized carbon scenario.

### Future Plans

More work will be done to expand the analysis to include electricity grid mix projections with a higher infiltration of renewables. Further, a more dynamic modeling will be implemented to reflect the PEV emissions profile using on-peak and off-peak electricity. A comparison of the regional sales of PEVs currently sold in the United States, compared to the sales projected out to 2035 by the U.S. Energy Information Administration, will help validate whether forecasting has held true in the market.

### Expected Outcomes

- Research in life cycle modeling of fuel economy and GHG standards and labels for PHEVs, which will be incorporated in the Sustainable Energy Systems curriculum
- Recommendations for vehicle fuel economy standards and labels, which will be shared with the EPA
- Long-term analysis of PEV standards policy to determine the impacts of changes to the electrical grid through time
- Strong collaborative relationship between the U.S.-China Clean Energy Research Center and the EPA, which develops new fuel economy and GHG standards
- A joint U.S./China wiki for collaborative data and modeling sharing among researchers
- Sharing of research outcomes with industry partners in the automotive sector that have a keen interest in future vehicle GHG standards

## Energy Systems Analysis, Technology Roadmaps, and Policy

## Fleet Modeling on China's In-use Vehicle Fleet

Joint Project

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
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*Research Objective*

This project will analyze China's in-use vehicle fleet, including the impact of the high vehicle fleet growth rates anticipated in China on the deployment rates of clean vehicle (CV) technologies. Researchers will develop a fleet model for China and use it to compare future deployment rates, growth scenarios, overall energy consumption, and greenhouse gas emissions with findings from the U.S. fleet model.

*Technical Approach*

- Build a fleet model to characterize future Chinese light-duty vehicle (LDV) energy demand, fuel demand, and carbon dioxide (CO<sub>2</sub>) emissions
- Gather data on vehicle characteristics (weight, power, fuel consumption, etc.)

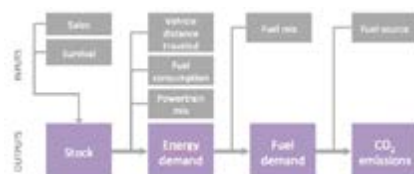


Figure 1: Fleet model diagram.

and perform quantitative analysis of vehicle technology between different model years, companies, and company types. This can inform potential means and likelihood of achieving future fuel consumption targets

- Incorporate further flexibility and detail into the fleet model by dividing rural and urban fleets (the majority of LDV vehicles are urban) and/or noting differences for regions, further alternative fuels, powertrains, etc.

*Significant Results*

The main results of this project include projections for LDV energy demand, fuel demand, and CO<sub>2</sub> emissions. Specifically, lower vehicle fuel consumption, modest alternative powertrain adoption, and lower travel demand per vehicle in the reference scenario could

stabilize Chinese LDV energy demand after 20 years (see black line in Figure 2).

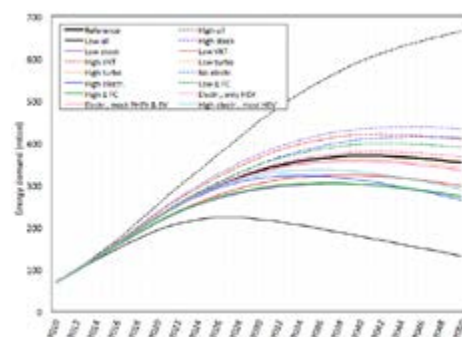
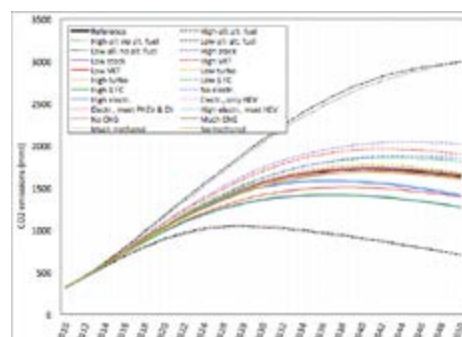


Figure 2: Chinese LDV energy demand (million tons of oil equivalent [mtoe]).

These reference scenario results indicate that future maximum Chinese fuel demand could tangent maximal U.S. LDV transportation energy demand from circa 2010.

The most significant drivers to lower future Chinese LDV energy demand and CO<sub>2</sub> emissions below reference scenario results are vehicle stock, vehicle fuel consumption, and hybrid electric/electric vehicles.

Figure 3: China LDV CO<sub>2</sub> emissions (million metric tons [mmt] CO<sub>2</sub>).

The analysis also identified potentially significant political implementation barriers for many policies that would impact future LDV energy consumption. Specifically, if the government level of policy announcement and implementation differ, policy success may be compromised. Overcoming these barriers is a necessary step to effecting the change that will allow future energy demand to stabilize.

*Future Plans*

In the future, this project will continue to pursue the following activities:

- Rigorously compare the Chinese LDV energy demand results with fleet model studies from other countries (the United States primarily, Europe and Japan thereafter)
- Compare vehicle technology characteristics and incorporate results into fleet model scenarios
- Explore drivers of vehicle ownership (urban versus rural, income, etc.)

*Expected Outcomes*

- Data analysis and a validated in-use fleet model for light-duty transportation in China (complete)
- Scenario analysis on different strategies to reduce vehicle energy demand (complete)
- Quantitative analysis on passenger car vehicle characteristics and technologies in China (in progress)
- Comparison of rural-urban ownership patterns and how this affects future Chinese LDV energy demand
- More rigorous analysis of policy options to control LDV energy demand and emissions in China. Compare CV technologies with other policy options

# Electricity and Material Sourcing Scenario Analyses to Guide Vehicle Technology Strategies

Cooperative Project (U.S.)

U.S. Research Team Lead	China Research Team Lead
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U.S. Partners	China Partners
<ul style="list-style-type: none"><li>Ford Motor Company</li><li>General Motors</li></ul>	<ul style="list-style-type: none"><li>Tsinghua University</li><li>China Automotive Technology Research Center</li></ul>

Research Objective

The project is conducting materials sourcing studies. The project team will gain understanding of the impact of the source of vehicle component materials on life cycle energy and emissions. The project will also develop an enhanced electrical grid model to include future fueling scenarios with renewable energy and lower carbon-based electricity strategies. The grid model will be applicable to other projects, such as Project 6.3. Based on the electrical grid model, researchers will evaluate renewable electricity scenarios that include renewable portfolio standards within the United States in the context of plug-in hybrid electric vehicle (PHEV) penetration. The team will also further analyze the impact of alternative design and technology strategies for improving PHEV performance across electric grid scenarios. Finally, this project will provide guidance on vehicle technology strategies by integrating the enhanced electrical grid model and materials sourcing scenarios within a single cohesive framework.

Technical Approach

- Generate a detailed life cycle model of primary aluminum produced within the United States that contains a high level of spatial resolution; evaluate primary aluminum production at each U.S. smelter, applying varying electricity allocation boundaries (power control area boundaries, state boundaries, North American Electric Reliability Corporation [NERC] boundaries, etc.). Varying boundaries are needed because electrons cannot be tracked
- Evaluate the impact of vehicle lightweighting via aluminum using a detailed vehicle simulation model (Autonomie), include production emissions to compare life cycle impacts of aluminum against conventional steel

Significant Results

The project created a high-resolution life cycle model of primary aluminum production in the United States. This model details the life cycle greenhouse gas (GHG) emissions for each of the nine primary U.S. aluminum smelters. The model uses a cradle-to-gate approach, accounting for all emissions associated with creating an aluminum ingot that would then be used in a manufacturing process.

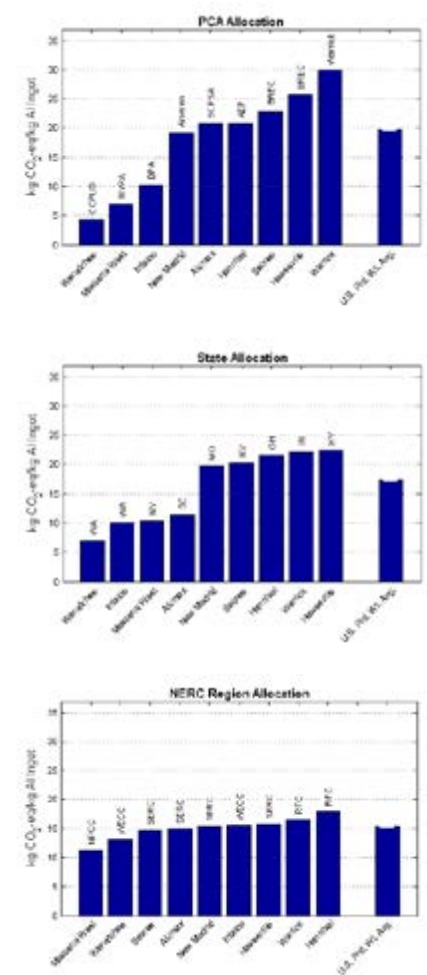
Project researchers applied known rates of GHG emissions from electrical utilities at varying regional scales. This is important because the electricity market cannot be simply allocated, with perfect knowledge, to any one regional scale because of the large amounts of trading that occurs between power control areas (PCAs), states, and NERC regions. The allocation protocols (or regional levels) examined in this study are the PCA, state, eGRID sub-region, NERC, and the United States.

Results from the aluminum sourcing analysis suggest that allocation protocols have a significant impact on the conclusions that can be drawn regarding a smelter's GHG performance. Increasing the geographic region of interest tends to normalize smelter GHG emissions and obscure the important variances that exist between the different smelters.

Researchers used Autonomie to simulate a PHEV, similar to the 40-mile all-electric-range Chevrolet Volt, over U.S. Environmental Protection Agency (EPA) drive cycles to determine on-road vehicle GHG emissions. The team also used the EPA eGrid model to determine use phase GHG emissions. These results were combined with upstream GHG emissions from Argonne National Laboratory's Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model and the results of the aluminum study; the pooled findings were used to determine the benefit of PHEV lightweighting.

The project team also developed a lightweight model of PHEV by substituting a PHEV aluminum hood for a steel hood. Simulation results suggest that, even with 100% primary

aluminum, lightweighting performs no worse than a conventional steel hood, suggesting that aluminum could realize a full life cycle GHG benefit for PHEVs, considering recycling.



Figures 1, 2, and 3. GHG emissions by differing allocation protocols.

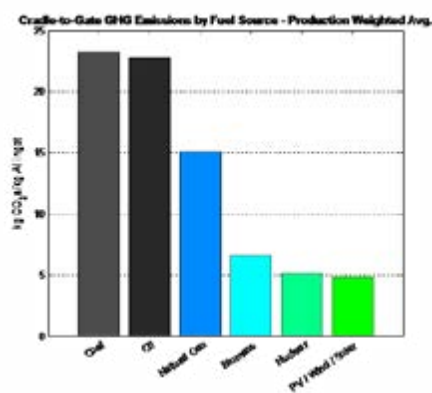


Figure 4. GHG emissions by electricity fuel source.

### Future Plans

Future work includes the application of several end-of-life scenarios to the life cycle model, sensitivity analyses of aluminum production, and the development of a reduced order electrical grid model.

### Expected Outcomes

- Recommendations on lightweighting's effectiveness under different grid scenarios
- Analysis from the material sourcing model, which will provide industry with a strategic method for identifying how material source location can be used to reduce vehicle life cycle impacts
- A reduced order electrical grid model for emissions calculation in the context of life cycle assessment

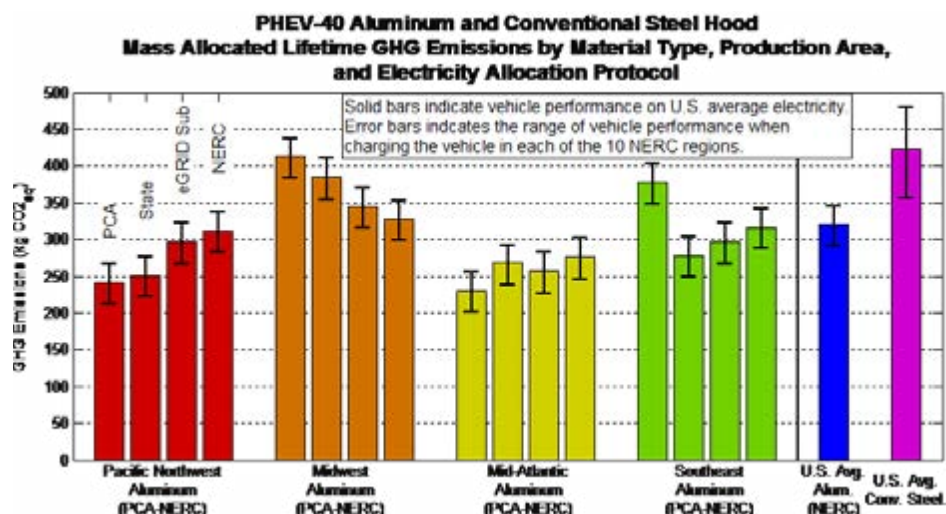


Figure 5. GHG emissions of a lightweighted vehicle.



# Appendix H: Acronym List

25DMH	2,5-dimethylhexane	CDI	Capacitive deionization	ECCE	Energy Conversion Congress and Exposition
3D	Three-dimensional	CEF	U.S.-China Clean Energy Forum	ECM	Equivalent circuit model
4WID-EV	Four-wheel independent-drive electric vehicles	CERC	U.S.-China Clean Energy Research Center	EELS	Electron energy loss spectroscopy
A	Amperes	CFD	Computational fluid dynamics	EFR	Entrained flow reactor
A-USC	Advanced ultra supercritical	CFS	Complex fenestration system	EGR	Exhaust gas recirculation
ACTC	Advanced Coal Technology Consortium	CFPP	Coal-fired power plant	EMI	Electromagnetic interference
AEP	American Electric Power	CGS	CO <sub>2</sub> geological storage	EMF	Electromotive force
AFM	Atomic force microscopy	CHP	Combined heat and power	EMS	Ethylmethanesulfonate
AHSS	Advanced high-strength steel	CI	Compression-ignition	EOR	Enhanced oil recovery
APU	Auxiliary power unit	CNF	Carbon nanofiber	EPA	U.S. Environmental Protection Agency
ASHRAE	American Society of Heating, Refrigeration, and Air Conditioning Engineers	CO <sub>2</sub>	Carbon dioxide	EPE	Electro-plastic effect
ATDC	After top dead center	COIR	Cell Ohmic internal resistance	EPR	Electron paramagnetic resonance
AVESTAR	Advanced virtual energy simulation training and research	COMO	Combustion model at B&W	Er	Reduced modulus
B0	0% biofuel blend	CPECC	China Power Engineering Consulting Group Corporation	EV	Electric vehicle
B100	100% biofuel blend	CR	Contact resistance	eV	Electron volts
BD	Biodiesel	CRADA	Cooperative research and development agreement	FCS	Full chain system
BEE	Building Energy Efficiency	CV	Clean vehicles	FEM	Finite element method
BTU	British thermal unit	CVC	Clean Vehicles Consortium	FF-EFR	Flat flame entrained flow reactor
B&W	Babcock & Wilcox	DER-CAM	Distributed Energy Resources Center Customer Adoption Model	FRPC	Fiber-reinforced polymeric composite
CA	Crank angle	DeST	Designer's simulation toolkit	FSW	Friction stir welding
CAD	Computer-aided design	DFA	Design for assembly	FUDS	Federal urban driving cycle
CAE	Computer-aided engineering	DFM	Design for manufacturing	FURN	Furnace code at HUST
CAER	Center for Applied Energy Research	DFT	Density field theory	FY	Fiscal year
CAERI	Chinese Automotive Engineering Research Institute	DFT+U	DFT with Hubbard augmentation of d-electrons	GHG	Greenhouse gas
CAFE	Corporate average fuel economy	DGAT	Diglyceride acyltransferase	GHX	Ground heat exchangers
CAN	Controller area network	DME	Dimethoxyethane	GREET	Argonne National Laboratory's greenhouse gases, regulated emissions, and energy use in transportation model
CATARC	China Automotive Technology & Research Center	DOE	U.S. Department of Energy	GSHP	Ground source heat pump
CCS	Carbon capture and storage	DSCC	Dynamic Systems and Control Conference	HA	Hazard analysis
CCUS	Carbon capture, use and storage	E	Energy	HCCI	Homogeneous charge compression ignition
CDCS	Charge-depleting charge-sustaining	E85	85% ethanol fuel blend	HEV	Hybrid electric vehicle
		EC	Ethylene carbonate	HIT	Harbin Institute of Technology

HOMO	Highest occupied molecular orbital	mmt	Million metric tons	R&D	Research and development
HPCC	High premixed compression combustion	MOHURD	China Ministry of Housing and Urban-Rural Development	RCSI	Retrospective cost-based subsystem identification
HSS	High-strength steels	MOST	China Ministry of Science and Technology	RCx	Retro commissioning
HUST	Huazhong University of Science and Technology	MPa	Megapascal	RFS	Renewable fuel standard
HVAC	Heating, ventilation, and air conditioning	mtoe	Million tons of oil equivalent	RFS2	Modified renewable fuel standard
IC	Incremental capacity	MW	Megawatt	RI	Rayleigh Index
ICA	Incremental capacity analysis	MWe	Megawatt electrical	rpm	Revolutions per minute
ICC	Integrated chassis control	MWth	Megawatt thermal	SaaS	Software as a service
ICE	Internal combustion engine	mV	Millivolts	SBS	Small boiler simulator
ICV	Internal combustion vehicle	n-BCH	n-butylcyclohexane	SEI	Solid electrolyte interface
IECC	International energy conservation code	NDP	Neutron depth profiling	SI	Spark ignition
IFC	International fire code	NEA	China National Energy Administration	SNG	Synthetic natural gas
IGCC	Integrated gasification combined cycle	NERC	North American Electricity Reliability Corporation	SOC	State of charge
IP	Intellectual property	NETL	National Energy Technology Laboratory	SOC	Start of combustion
ISO	International standards organization	NIST	National Institute of Standards and Technology	SOF	State of function
ITM	Ion transport membrane	NRAP	National Risk Assessment Partnership	SOH	State of health
ITS	Intelligent transportation systems	NRDC	Natural Resources Defense Council	SOI	Starts of injection
K	Degrees Kelvin	NVH	Noise vibration and harshness	SPE	Society of Plastic Engineers
kW	kilowatt	OCV	Open-circuit voltage	S&T	Science and technology
LBNL	Lawrence Berkeley National Laboratory	ORNL	Oak Ridge National Laboratory	SThEM	Scanning thermoelectric microscopy
LDV	Light-duty vehicle	ORR	Oxygen reduction reaction	SVR	Support vector regression
Li	Lithium	OSU	The Ohio State University	TAG	Triacylglyceride
Li-P-S	Lithium-Phosphorus-Sulfur	PBR	Photobioreactors	THU	Tsinghua University
LMI	Linear matrix inequalities	PCA	Power control area	TMP	Technology Management Plan
LS-DYNA	General-purpose finite element program by the Livermore Software Technology Corporation	PCC	Post-combustion capture	TRIP	Transformation-induced plasticity
LTC	Low temperature combustion	PEV	Plug-in electric vehicle	UHSS	Ultra-high-strength steels
M	Molar	PHEV	Plug-in hybrid electric vehicle	UM	University of Michigan
MB	Methyl butanoate	PI control	Proportional-integral control	USC	Ultra supercritical
MCH	Methyl cyclohexane	pKa	Acid dissociation constant	V	Volts
MD	Methyl decanoate	PMSM	Permanent magnet synchronous motor	V2G	Vehicle-to-grid
MDHP	Methyl decanoate/n-heptane	POIR	Pseudo-Ohmic internal resistance	VARTM	Vacuum assisted resin transfer molding
MEA	Monoethanolamine	PRC	People's Republic of China	VLEB	Very low energy building
Mg	Magnesium	PV	Photovoltaic	W	Watt
MIT	Massachusetts Institute of Technology	Q	Battery charged capacity	WebOpt	Low energy building optimization web service
		R	Radicals	WVU	West Virginia University
				XANES	X-ray absorption near-edge spectroscopy
				xEV	Electric drive vehicle
				ZT	Dimensionless figure of merit



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