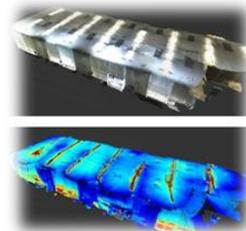


# ARPA-E Impacts:

*A Sampling of Project Outcomes, Volume II*





Dear Colleagues,

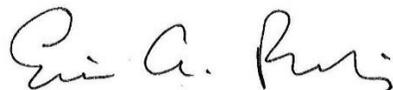
The Advanced Research Projects Agency-Energy (ARPA-E) is demonstrating that a collaborative model has the power to deliver real value. The Agency's first compilation booklet of impact sheets, published in 2016, began to tell the story of how ARPA-E has already made an impact in just seven years—funding a diverse and sophisticated research portfolio on advanced energy technologies that enable the United States to tackle our most pressing energy challenges. One year later our research investments continue to pay off, with a number of current and alumni project teams successfully commercializing their technologies and advancing the state of the art in transformative areas of energy science and engineering.

There is no single measure that can fully illustrate ARPA-E's success to date, but several statistics viewed collectively begin to reveal the Agency's impact. Since 2009, ARPA-E has provided more than \$1.5 billion in funding for 36 focused programs and three open funding solicitations, totaling over 580 projects. Of those, 263 are now alumni projects. Many teams have successfully leveraged ARPA-E's investment: 56 have formed new companies, 68 have partnered with other government agencies to continue their technology development, and 74 teams have together raised more than \$1.8 billion in reported funding from the private sector to bring their technologies to market.

However, even when viewed together, those measures do not capture ARPA-E's full impact. To best understand the Agency's success, the specific scientific and engineering challenges that ARPA-E project teams have overcome must be understood. This booklet provides concrete examples of those successes, ranging from innovations that will bear fruit in the future to ones that are beginning to penetrate the market as products today. Importantly, half of the projects highlighted in this volume stem from OPEN solicitations, which the agency has run in 2009, 2012, and 2015. ARPA-E's OPEN programs are an extraordinary opportunity for the R&D community to challenge ARPA-E in areas of technology not covered by the agency's focused technology programs.

Please share this report with your colleagues—we hope to encourage innovative scientists and engineers to continue to engage us with their ideas and consider joining our team as a Program Director, Fellow, or Tech-to-Market Advisor.

Sincerely,



Eric Rohlifing  
Acting Director of ARPA-E  
February 10, 2017



# TABLE OF CONTENTS

## DESCRIPTIONS OF ARPA-E'S PROGRAMS..... 3

### TRANSPORTATION FUELS..... 7

North Carolina State University and University of Massachusetts (PETRO) – Engineering the Optimized Biofuel Crop .....	8
University of Illinois (PETRO) – Oilcane: An Ideal Bioenergy Feedstock .....	12
Agrivida (OPEN 2009) – Engineering the Optimized Biofuel Crop .....	15
Massachusetts Institute of Technology (Electrofuels) – Liquid Transportation Fuel from Electricity and CO <sub>2</sub> .....	18
Dioxide Materials (OPEN 2012) – Converting Carbon Dioxide into Fuel .....	21
Lanzatech (REMOTE) – Cheaper, Faster Waste-Gas Fermenters for Fuels and Chemicals .....	24
Bio2Electric (Ecocatalytic) (OPEN 2012) – Flameless Combustion: Chemical Looping Ethane to Ethylene.....	27

### POWER GENERATION AND DISTRIBUTION ..... 30

RTI International (IMPACCT) – Carbon Capture with Water-Free Solvents.....	31
Lawrence Berkeley National Laboratory/University of California, Berkeley (IMPACCT) – Novel Metal-Organic Framework Sorbents for Carbon Capture.....	33
General Electric (OPEN 2012) – Back to the Future, for the Electric Power Grid .....	37
University of California, Berkeley (OPEN 2012) – Precise, Time Synchronized Distribution Grid Measurements	40
Brown University (OPEN 2012) – Self-Optimizing River and Tidal Power Conversion Devices.....	44
Integral Consulting (OPEN 2012) – Low-Cost, Real-Time Wave-By-Wave Assessment Tool .....	47
Otherlab (OPEN 2012) – Pneumatically-Actuated PV Tracking System Reduces Cost and Improves Reliability.....	50
Glint Photonics (OPEN 2012) – Low-Power Microscale Tracking for Low-Profile Daylighting.....	53

### BUILDING, TRANSPORTATION, AND INDUSTRIAL EFFICIENCY..... 56

Utah State University (AMPED) – Cell-Level Control in Large Battery Packs .....	57
General Electric (AMPED) – Getting the Best from a Battery .....	60
Otherlab (MOVE) – Intestine-Structured Gas Storage .....	63
United Technologies Research Center (MOVE) – Flat, Modular Tank Technology for Natural Gas Vehicles .....	66
Massachusetts Institute of Technology (HEATS) – Advanced Thermal Battery for Climate Control.....	68
University of Texas, Austin (OPEN 2012) – Low Cost Voltage-Controlled Window Can Be Tuned to Block Visible and/or Infrared Light.....	71
University of California, Berkeley (OPEN 2012) – Fast, Automated Building Energy Auditing .....	75
iBeam Materials (SWITCHES) – Low-Cost LEDs on Flexible Metal Tapes .....	78
Alcoa (METALS) – Reimagining Aluminum Manufacturing .....	81
University of Utah ( METALS) – A Thermal Pathway to Low Cost Titanium Powder.....	84



## DESCRIPTIONS OF ARPA-E'S PROGRAMS

Acronym	Title	Year	Brief Description
<b>ADEPT</b>	Agile Delivery of Electric Power Technology	2010	Power Conversion Efficiency: Wide band-gap semiconductors for high-power, high-current applications
<b>ALPHA</b>	Accelerating Low-Cost Plasma Heating and Assembly	2014	Fusion energy, focused on intermediate density regime, reducing the cost of experimental tests for fusion energy
<b>AMPED</b>	Advanced Management and Protection of Energy Storage Devices	2012	Battery storage, primarily for EV. Addressing efficiency from perspective of the overall battery pack with new approaches to the battery management system. Strong DoD engagement
<b>ARID</b>	Advanced Research in Dry-Cooling	2015	Developing technology to protect power plant efficiency under water constraints - More efficient 'dry-cooling'
<b>BEEST</b>	Batteries for Electric Energy Storage in Transportation	2010	All aspects of battery design and materials, supporting a large amount of alternative battery chemistry work (supplemented by project awards under OPEN 2009 and 2012)
<b>BEETIT</b>	Building Energy Efficiency Through Innovative Thermodevices	2010	Lower energy approaches to heating, ventilation and air conditioning (HVAC). Some projects funded by DoD
<b>CHARGES</b>	Cycling Hardware to Analyze and Ready Grid-Scale Electricity Storage	2014	Two test sites to allow grid-scale batteries to be validated under realistic grid operation conditions
<b>DELTA</b>	Delivering Efficient Local Thermal Amenities	2014	Local thermal management for comfort of individuals, goal to reduce overall AC costs by allowing less stringent building-wide AC
<b>ELECTROFUELS</b>	Microorganisms for Liquid Transportation Fuel	2010	Exploratory development of fuel productions by organisms that directly use electric charge as an energy source

Acronym	Title	Year	Brief Description
<b>ENLITENED</b>	Energy-Efficient Light-Wave Integrated Technology Enabling Networks that Enhance Datacenters	2016	Integrated photonic interconnects and novel switching networks for more energy efficient manipulation and movement of data
<b>FOCUS</b>	Full Spectrum Optimized Conversion and Utilization of Sunlight	2014	Solar energy approaches that capture both PV and thermal energy, including spectrum splitting to different collectors and development of PV cells that can work at the high T of thermal collection
<b>GENI</b>	Green Electricity Network Integration	2011	Electric power network - Power flow controllers & software to allow more effective integration of renewables
<b>GENSETS</b>	Generators for Small Electrical and Thermal Systems	2015	Distributed power generation - Low-cost, small scale generators for combined heat and power
<b>GRIDS</b>	Grid Scale Rampable Intermittent Dispatchable Storage	2010	Stationary storage, including grid-scale batteries, flow-batteries, and other approaches such as flywheels. Battery portfolio supplemented through OPEN 2009 and 2012 projects
<b>GRID DATA</b>	Generating Realistic Information for the Development of Distribution and Transmission Algorithms	2015	Development of realistic, open-source models of transmission and distribution grids to support advanced work on optimization and control algorithms
<b>HEATS</b>	High Energy Advanced Thermal Storage	2011	Thermal energy storage, including use of waste heat and storage of heat from concentrated solar and from nuclear power plant
<b>IMPACCT</b>	Innovative Materials and Process for Advanced Carbon Capture Technologies	2010	Carbon capture for emissions from coal plants, supplemented by project awards under OPEN 2009 and 2012
<b>IONICS</b>	Integration and Optimization of Novel Ion Conducting Solids	2016	Improving the properties of solid ion conductors for batteries, fuel cells, and other electrochemical devices
<b>METALS</b>	Modern Electro/Thermochemical Advances in Light Metal Systems	2013	Efficient production and recycling of Al, Mg, Ti – Lower cost and energy use to support vehicle light-weighting

Acronym	Title	Year	Brief Description
<b>MONITOR</b>	Methane Observation Networks with Innovative Technology to Obtain Reductions	2014	Sensing methane and localizing the leak point(s) economically enough for routine use by producers
<b>MOVE</b>	Methane Opportunities for Vehicular Energy	2012	New forms of storage for natural gas that will reduce volume of tanks or allow them to be integrated into the body of the vehicle
<b>MOSAIC</b>	Micro-Scale Optimized Solar-Cell Arrays with Integrated Concentration	2015	Developing compact solar concentration onto high-efficiency cells while also maintaining capture of diffuse sunlight
<b>NEXTCAR</b>	Next-Generation Energy Technologies for Connected and Automated On-Road Vehicles	2016	Vehicle and powertrain control technologies to reduce automotive energy use
<b>NODES</b>	Network Optimized Distributed Energy Systems	2015	Developing control algorithms to create effective grid storage through distributed demand response, e.g. water heaters
<b>PETRO</b>	Plants Engineered to Replace Oil	2011	Modification of plants to directly produce fuel-ready hydrocarbons
<b>RANGE</b>	Robust Affordable Next -Generation Energy Storage Systems	2013	Battery designs that improve the overall energy density and cost effectiveness of the battery system by using safer materials
<b>REACT</b>	Rare Earth Alternatives in Critical Technologies	2011	Materials and motor design approaches that provide options for continued high-efficiency in the event of rare-earth shortages
<b>REBELS</b>	Reliable Electricity Based on Electrochemical Systems	2014	Fuel cells designed for use in distributed power generation (down to residential scale)
<b>REFUEL</b>	Renewable Energy to Fuels through Utilization of Energy-Dense Liquids	2016	Energy-dense liquid fuels from water and CO <sub>2</sub> and/or N <sub>2</sub> from air powered by renewable electricity
<b>REMOTE</b>	Reducing Emissions using Methanotrophic Organisms for Transportation Energy	2013	Biological conversion of methane to fuels
<b>ROOTS</b>	Rhizosphere Observations Optimizing Terrestrial Sequestration	2016	Biofuel plant root phenotyping for improved growth properties and atmospheric carbon sequestration

Acronym	Title	Year	Brief Description
<b>SHIELD</b>	Single-Pane Highly Insulating Efficient Lucid Designs	2016	Insulating window materials with excellent optical quality which prevent condensation, for cost-effective retrofits or replacements
<b>SOLAR ADEPT</b>	Solar Agile Delivery of Electrical Power Technology	2011	Improved electrical interconnects for integrating solar power with the grid
<b>SWITCHES</b>	Strategies for Wide Bandgap, Inexpensive Transistors for Controlling High-Efficiency Systems	2013	Devices to improve Energy Efficiency for electric motors
<b>TERRA</b>	Transportation Energy Resources from Renewable Agriculture	2015	More rapid development of sustainable biofuels crops through sensing, robotics, informatics and genetics for advanced phenotyping of energy crops
<b>TRANSNET</b>	Traveler Response Architecture using Novel Signaling for Network Efficiency in Transportation	2015	Control architectures and traveler incentives for energy optimization of urban networks

# TRANSPORTATION FUELS

## Overview:

ARPA-E has invested in novel ways to synthesize energy dense liquid fuels as alternatives to petroleum-based fuels that power most vehicles in the United States. A diverse set of alternative feedstocks have been developed or used such as biomass, carbon dioxide, and natural gas. The ultimate goal is to develop drop-in replacements for petroleum-based fuels, reducing vulnerability to imports, and greatly reducing net greenhouse gas (GHG) emissions. This is an area where rapid advances in genomics and bioengineering are creating a wealth of new opportunities for innovative new approaches.

Today's vision for cost-competitive domestically produced biofuels is hampered by a number of issues, one of which is that today's fuel-rich crops do not yet provide enough of a step up (based on energy yield per unit area) to be an economically compelling alternative for production of transportation fuel at scale. The "Plants Engineered to Replace Oil" or PETRO program (2011) aimed to redirect the processes for energy and carbon dioxide capture in plants toward fuel production. This would create dedicated energy crops that serve as a domestic alternative to petroleum-based fuels and deliver more energy per acre with less processing prior to the pump. Other projects from OPEN funding solicitations offer additional approaches to more energy-rich biofeedstocks.

Another approach to biologically derived fuels is to utilize microorganisms that are capable of producing energy not from the sun or from consuming sugar, but rather from inorganic energy sources such as hydrogen or electricity to power the conversion of CO<sub>2</sub> to fuels. The Electrofuels program (2010) advanced technologies that provide an option to "recycle" CO<sub>2</sub> and help close the emissions-loop for transportation. Complementary OPEN projects have explored the use of chemical or electrochemical processes to convert CO<sub>2</sub> into chemicals and fuels.

The current abundance of domestic natural gas offers opportunities for its use in the transportation sector; however, the inherently low energy density of natural gas makes it a relatively poor substitute for petroleum-based liquid fuels. Conventional approaches to the conversion of natural gas to liquid fuels rely on chemical processes that are only cost-competitive at very large scales and are not applicable to smaller scale sources, such as natural gas that is "stranded" in production fields or biogas from landfills. Projects in the "Reducing Emissions using Methanotrophic Organisms for Transportation Energy," or REMOTE program (2013) are examining biological approaches for converting methane to liquid fuels that can be implemented cost effectively at small scales. Complementary projects from OPEN solicitations have also used chemical or electrochemical methods for the efficient and cost-effective conversion of methane and other hydrocarbons to more valuable chemicals.

The following projects provide a good sampling of the diversity of feedstocks for and synthetic approaches to low-GHG fuels for the transportation sector:

- North Carolina State University and University of Massachusetts (PETRO) – Engineering the Optimized Biofuel Crop
- University of Illinois (PETRO) – Oilcane: An Ideal Bioenergy Feedstock
- Agrivida (OPEN 2009) – Engineering the Optimized Biofuel Crop
- Massachusetts Institute of Technology (Electrofuels) – Liquid Transportation Fuel from Electricity and CO<sub>2</sub>
- Dioxide Materials (OPEN 2012) – Converting Carbon Dioxide into Fuel
- Lanzatech (REMOTE) – Cheaper, Faster Waste-Gas Fermenters for Fuels and Chemicals
- Bio2Electric (Ecocatalytic) (OPEN 2012) – Flameless Combustion: Chemical Looping Ethane to Ethylene

# ENGINEERING THE OPTIMIZED BIOFUEL CROP

Updated: January 10, 2017

<b>PROJECT TITLE:</b>	Jet Fuel From Camelina Sativa: A Systems Approach	Developing a Dedicated High-Value Biofuels Crop
<b>PROGRAM:</b>	Plants Engineered to Replace Oil (PETRO)	
<b>AWARD:</b>	\$8,556,904	\$3,751,152
<b>PROJECT TEAM:</b>	North Carolina State University (Lead); Metabolix	University of Massachusetts (Lead); Washington State University; Metabolix
<b>PROJECT TERM:</b>	January 2012 – December 2016	January 2012 – December 2015
<b>PRINCIPAL INVESTIGATOR (PI):</b>	Dr. Heike Sederoff	Dr. Danny Schnell

## TECHNICAL CHALLENGE

Biofuels offer renewable alternatives to petroleum-based fuels that can reduce net greenhouse gas (GHG) emissions dramatically. Today's vision for cost-competitive domestically produced biofuels must address challenges in sustainable production of bio-energy crops, and cost-effective production of drop-in fuels for demanding applications such as air transportation. Sustainability requires crops with high yields per land area, the ability to use land that is less useful for food crops, and reduced agronomic inputs (e.g. water, fertilizer, etc.). Cost-effective production of drop-in fuels requires biomass products that need limited processing, for which oil-rich crops are promising. However, existing oil-rich crops do not provide enough energy yield per land area to be a cost-effective alternative for production of transportation fuel at scale. Traditional breeding approaches in the major row crops produce between 1-2% increases in yield annually, which is insufficient to generate the yields needed for economically viable drop-in fuels.

## TECHNICAL OPPORTUNITY

Recent advances in synthetic biology and decreased cost of custom DNA synthesis now allow complex metabolic pathway engineering in plants. These technologies are enabling researchers to incorporate novel biosynthetic pathways into both model plants and row crops for the field. Camelina sativa is a promising oilseed crop that can grow in geographies that traditional row crops do not, has a short generation time, and requires low agronomic inputs. A rapid and efficient genetic transformation method was previously developed for Camelina, which allows researchers to engineer complex traits into the plant.

## INNOVATION DEMONSTRATION

Under the Plants Engineered To Replace Oil (PETRO) program, ARPA-E funded projects at North Carolina State University (NCSU) and the University of Massachusetts (UMass) focused on engineering Camelina to dramatically increase the oil yield of the crop, and the composition of the oil to be a better fuel. The two projects had similar goals, but used different biological approaches. UMass teamed with Washington State University (WSU) and Metabolix Inc., a biotechnology company that is a pioneer in the field of metabolic engineering. NCSU added Metabolix as a commercial partner in 2015. As their projects matured, the two teams developed a collaboration to combine the synergistic approaches from each of their projects.

### NCSU Project

The NCSU team's goal was to double the seed-yield of the crop through increased photosynthetic efficiency and channeling the energy captured through photosynthesis to oil production. NCSU identified numerous novel plant genes and metabolic pathways to increase carbon dioxide (CO<sub>2</sub>) fixation, reduce photorespiratory energy and carbon loss, increase yield, and shorten the growth cycle of Camelina. The lines engineered with these traits that showed increased biomass and seed yields over multiple generations in the greenhouse were selected for further characterization and development. One of the most promising targets are cell wall invertase inhibitors (CWIs), which regulate the transport of sugar from the photosynthetically active tissues (like leaves) in the plant to the non-green roots, flowers and seeds. NCSU engineered this target gene to increase the levels of sugar available for biomass production and seed yield, which led to

Camelina with higher vegetative biomass (>20%), higher rates of photosynthesis and increased seed yield (40-80%) compared to wild type (WT) control (Figure 1). Another pathway reduces the loss of CO<sub>2</sub> from photorespiration during photosynthesis. Camelina plants expressing enzymes for this pathway flower and set seed almost a week earlier than wild type plants without reducing yield. This is valuable to farmers because it allows them greater flexibility with sowing and harvesting. Flowering though, is very dependent on environmental conditions, so this phenotype requires testing under field conditions.

### UMass Project

The UMass team used alternative strategies to increase photosynthetic activity and seed yield. Primarily, UMass worked to introduce carbon-concentrating mechanisms into the plant's cells to increase the intracellular levels of CO<sub>2</sub>, and increase photosynthesis. UMass evaluated a number of metabolite transporters from microalgae and cyanobacteria in Camelina, and identified one that reliably increased biomass and seed yield in Camelina over multiple generations. The transporter functioned by increasing the availability of CO<sub>2</sub> within the cell to significantly increase the catalytic rate of CO<sub>2</sub> fixation by RuBisCO, and increased photosynthetic efficiency in the Camelina plants by 10-25% (Figure 2). In an initial small-scale field trial, Camelina lines expressing the transporter produced up to 75% more seed and increased oil yields than wild type plants (Figure 2).

The Camelina plants expressing components of the carbon concentrating mechanism also showed enhanced resistance to water stress (Figure 2), because the plants more efficiently fix CO<sub>2</sub> and can reduce gas exchange between leaves and the atmosphere.

### Collaborative Work

As the UMass metabolite transporter functioned through a distinct mechanism from NCSU's traits, ARPA-E encouraged the two teams to work together. NCSU and UMass stacked the transporter and cell wall invertase inhibitor together in Camelina and observed in the laboratory an additional 15% increase in vegetative biomass production and increased seed yield in the stacked lines compared to the parent line. Metabolix partnered with NCSU in 2015 to test promising Camelina lines from the NCSU and UMass programs in a field trial as a first step to incorporating the lines or traits into Metabolix's commercial pipeline. Due to Camelina's short lifecycle, homozygous seeds ready for field trials can be obtained within a year allowing for rapid field-testing of promising traits. Field trials were established in multiple locations in 2016, and are now underway to test the most promising Camelina traits from these two PETRO projects against Metabolix's existing high yielding Camelina varieties. At the end of the project period, the field data on the oil yields from the Camelina lines expressing the PETRO traits will be independently validated by Oak Ridge National Laboratory.

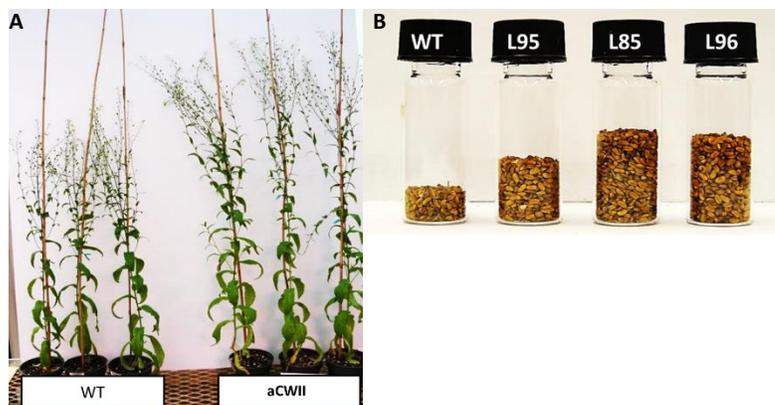


Figure 1: (A) Comparison of vegetative growth between WT and CWII plants, and (B) per plant seed yield of CWII transgenic Camelina lines (L95, L85, L96).

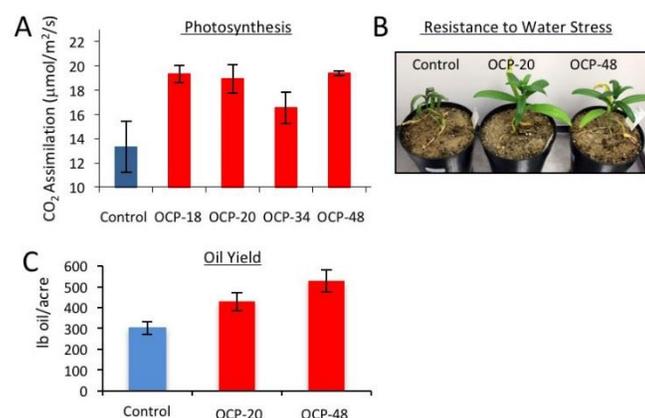


Figure 2: (A) Increased photosynthetic activity, (B) enhanced resistance to water stress, and (C) increased oil yields in Camelina transporter lines.

## PATHWAY TO ECONOMIC IMPACT

The key to the successful adoption of a new crop like Camelina is grower acceptance. NCSU produced economic models under ARPA-E support that show that increases in Camelina seed oil yield of 70%, which is the level of increase NCSU observed in the greenhouse with its traits, would more than triple farmers' profits. Figure 3 shows data for 67% and 133% increases in seed yield per acre as compared with the average of 2009-2013 profits from corn in the eastern and western corn belt. Although, in some regions Camelina yields are not sufficient to provide enough economic incentive to displace corn and soy acreage, Camelina can be grown in regions that are not well suited for these traditional crops. Following the field tests, NCSU will incorporate the new data into its techno-economic model to evaluate the economic potential as a biofuel feedstock.

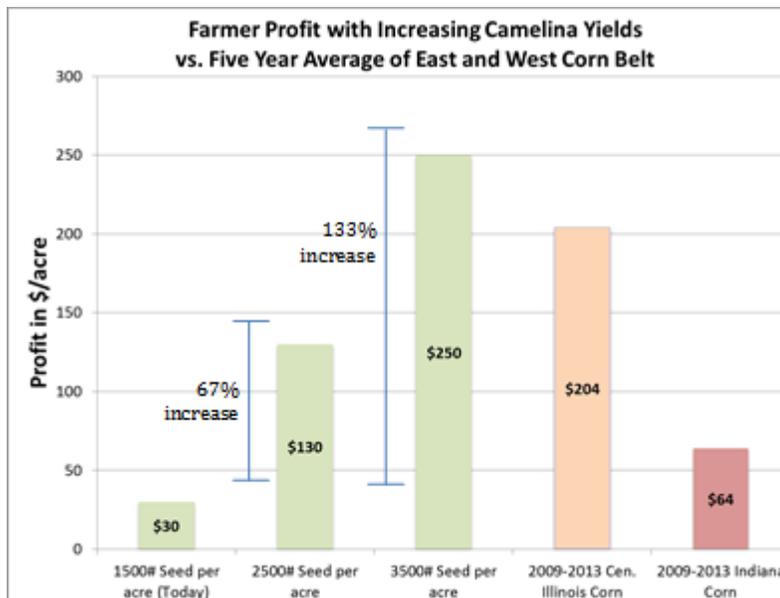


Figure 3: Modeled farmer profit with increasing Camelina yields (green bars) vs 5 year average profits from high productivity "corn only" farmland in the Eastern and Western cornbelt. Data sources: NC State economic model for Camelina; University of Illinois and Purdue University for 2009-2013 corn profits.

## ECONOMIC DEVELOPMENT

The pathway to economic impact for this project will be determined by the outcomes of the field trials in 2016, for which Metabolix has licensed the promising PETRO traits from UMass and NCSU. The successful traits will be moved into Metabolix's commercial Camelina varieties for further large-scale field trials. Continuing work to further improve Camelina yield will be supported in part by a \$2.5 million award to Metabolix and NCSU from the DOE BioEnergy Technology Office, covering activities to further develop Camelina lines with increased seed yield and oil content using a genome editing approach.

In addition to the Camelina work, using internal funding, Metabolix is also currently working to transfer select licensed traits into C3 row crops such as rice, canola and soybeans, while evaluating whether any of the traits will also increase yield in C4 crops, which include major row crops such as corn, sorghum, or sugar cane. The results of this analysis will guide future commercialization efforts and licensing/negotiations with major agricultural companies.

Metabolix will develop first markets for the NCSU/UMass traits in high-value feedstock market opportunities in the food, feed and fuel sectors. These select market segments will support the development expense of new plant feedstocks, facilitating their staged introduction into commodity markets.

## LONG-TERM IMPACTS

Success in the first-market strategy outlined above is expected to provide a foundation for future commercialization efforts in biofuels and advanced biofuels. Camelina derived jet fuel has been successfully tested by the U.S. Air Force, Navy, and by commercial airlines. The PETRO technology has the potential to make this approach economically competitive.

Furthermore, if the demonstrated large increases in yield do readily transfer into C3 and C4 row crops, this technology could make a major contribution towards increasing world food production while minimizing impacts on water, energy, and land resources.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

The NCSU team had 18 inventions and filed four patent applications, the UMass team had 10 inventions, and the combined NCSU and UMass team had one joint invention, for a total of 29 inventions and four patent applications.

The NCSU and UMass teams have published the scientific underpinnings of these technologies in the open literature. A list of scientific publications and patent applications is provided below:

## NCSU

"*Technoeconomic analysis of jet fuel production from hydrolysis, decarboxylation, and reforming of camelina oil*," R. Natelson, W. Wang, W. Roberts, K. Zering, *Biomass & Bioenergy*, Vol. 75, pg. 23-34, DOI: 10.1016/j.biombioe.2015.02.001, 2015.

"*A photorespiratory bypass increases plant growth and seed yield in biofuel crop Camelina sativa*." J. Dalal, H. Lopez, N. Vasani, Z. Hu, J. Swift, R. Yalamanchili, H. Sederoff, *Biotechnology for biofuels* 8.1, p. 1, 2015.

"*Tissue-specific production of limonene in Camelina sativa with the Arabidopsis promoters of genes BANYULS and FRUITFULL*," M. Borghi, D. Xie, *Planta*, 1;243(2):549-61, 2016

"*Overexpression of a synthetic insect-plant geranyl pyrophosphate synthase gene in Camelina sativa alters plant growth and terpene biosynthesis*." J. Xi, L. Rossi, X. Lin, D. Xie. *Planta*. 2016 Mar 29:1-6.

"*A novel gateway-compatible binary vector series (PC-GW) for flexible cloning of multiple genes for genetic transformation of plants*." J. Dalal, R. Yalamanchili, C. La Hovary, M. Ji, M. Rodriguez-Welsh, D. Aslett, S. Ganapathy, A. Grunden, H. Sederoff, R. Qu, *Plasmid*. 2015 Sep 30; 81:55-62.

## UMass

"*Transcriptome profiling of Camelina sativa to identify genes involved in triacylglycerol biosynthesis and accumulation in the developing seeds*," H. Abdullah, P. Akbari, B. Paulose, D. Schnell, W. Qi, Y. Park, A. Pareek, O. Dhankher, *Biotechnol Biofuels*, 9:136. doi: 10.1186/s13068-016-0555-5, 2016.

"*Genome and Transcriptome of Clostridium phytofermentans, Catalyst for the Direct Conversion of Plant Feedstocks to Fuels*," M. Coppi, J. Hayes, A. Tolonen, T. Warnick, W. Latouf, D. Amisano, A. Biddle, S. Mukherjee, N. Ivanova, A. Lykidis, M. Land, L. Hauser, N. Kyrpides, B. Henrissat, J. Lau, D. Schnell, G. Church, S. Leschine, J. Blanchard, *PLoS One* 10(6):e0118285. doi: 10.1371/journal.pone.0118285, 2015.

"*Involvement of a Bacterial Microcompartment in the Metabolism of Fucose and Rhamnose by Clostridium phytofermentans*," E. Petit, W. LaTouf, M. Coppi, T. Warnick, D. Currie, et al., *PLoS ONE* 8(1): e54337. doi:10.1371/journal.pone.0054337, 2013.

"*Biological conversion assay using Clostridium phytofermentans to estimate plant feedstock quality*," S. Lee, T. Warnick, S. Pattathil, J. Alvelo-Maurosa, M. Serapiglia, H. McCormick, V. Brown, N. Young, D. Schnell, L. Smart, M. Hahn, J. Pedersen, S. Leschine, S. Hazen, *Biotechnology for Biofuels* 5:5, 2012.

# OILCANE: AN IDEAL BIOENERGY FEEDSTOCK

Updated: February 6, 2017

**PROJECT TITLE:** Engineering Hydrocarbon Biosynthesis and Storage Together with Increased Photosynthetic Efficiency into the Saccharinae

**PROGRAM:** Plants Engineered to Replace Oil (PETRO)

**AWARD:** \$6,479,275

**PROJECT TEAM:** University of Illinois at Urbana-Champaign (Illinois) (Lead), the Universities of Nebraska and Florida, and Brookhaven National Laboratory

**PROJECT TERM:** February 2012 – March 2017

**PRINCIPAL INVESTIGATOR (PI):** Steven Long

## TECHNICAL CHALLENGE

Plant lipids offer a renewable alternative to fossil liquid fuels, providing an inexhaustible and sustainable source within the U.S. while reducing net greenhouse gas (GHG) emissions. However, there are concerns about land use and the agronomic inputs needed to harvest large quantities of biomass sustainably. Increasing the yield of bioenergy crops, and their energy density, addresses both economic and sustainability concerns, especially if the feedstock needs limited processing. Developing oil-rich crops that can yield economically viable drop-in fuels is of particular interest, but traditional breeding approaches, which in the major row crops produce 1-2% increases in yield annually, are insufficient to produce the gains needed.

## TECHNICAL OPPORTUNITY

Hybridization provides an opportunity to combine promising plant characteristics to create improved crops. Sugarcane is one of the most photosynthetically productive crops in the world and ethanol produced from cane sugar is cost competitive with gasoline. The yield of ethanol from sugarcane is almost twice that of corn grain on a per acre basis; however, sugarcane is a tropical plant and is not grown commercially in the United States outside the southern areas of Florida, Texas, and Louisiana. Miscanthus is a wild relative of sugarcane capable of hybridization with sugarcane, and is expected to confer some of its cold tolerance to the sugarcane-miscanthus (miscane) hybrids.

## INNOVATION DEMONSTRATION

The Illinois team proposed to develop a bioenergy crop capable of producing 17 times the amount of oil produced by an acre of soybean and twice the fuel yield as corn ethanol in the U.S. by engineering sugarcane to (1) increase cold tolerance; (2) increase photosynthetic efficiency; and (3) accumulate energy dense triacyl-glycerol (TAG) molecules instead of sugar. While the optimal energy cane plant would contain all three traits, the Illinois team was only able to characterize each trait separately due to the long generation time in producing transgenic sugarcane. The baseline for the work is commercial sugarcane, which typically yields 10-15% sugar by weight and no TAGs. Miscanthus, which was to be hybridized with sugarcane, does not produce sugar or TAG. It is currently being developed as a cellulosic feedstock.

Prior to the start of this project, the Illinois team had collected a number of Miscanthus plants from cold climates such as Siberia. These Miscanthus were capable of surviving freezing temperatures, while in contrast sugarcane does not typically recover when exposed to temperatures below 10°C. The Illinois team crossed the two varieties of plants to generate miscane hybrids, and observed that some of the hybrids were able to retain 70% of their photosynthetic activity when grown at 14°C, over twice that of the sugarcane parent. These hybrids also overwintered in field trials in Arkansas under conditions that completely inhibited sugarcane.

To further improve the efficiency of sugarcane, the Illinois team took advantage of its recently developed biophysical model of photosynthesis to identify transformed gene constructs predicted to improve photosynthetic activity and



Figure 1: Florida field trial of wild type and transgenic sugarcane.

carbon fixation. By overexpressing specific genes involved in the C4 photosynthesis pathway, Illinois and its partners increased the carbon fixation activity of sugarcane. In field tests (Figure 1), certain lines of transgenic sugarcane exhibited >50% increased photosynthetic activity compared to wild type cane (Figure 2), and this translated to an increase in biomass of almost 50% in one line. Increase in biomass will in turn increase sugar yield per acre compared to wild type plants, because the sugar content stays constant.

Illinois and its partners also introduced metabolic pathways responsible for TAG accumulation in the seeds of oilseed plants, and isolated sugarcane lines containing up to 8% TAG by dry weight in their leaves (Figure 3). This level is over 200-fold greater than observed in wild type cane. The transgenic plants did not show any negative impact on growth rate or overall plant health when grown in the greenhouse, and still accumulated similar levels of sugar as wild type plants. There was also a corresponding increase in total fatty acids in the plant, suggesting that there is still the potential to convert more fatty acids into TAG in the transgenic plants.

The cold tolerance and increased photosynthesis traits have the potential to increase the yield of one of the most productive crops on the planet and deploy it in the U.S. However, the oil trait, which would convert the sugar into a more energy-dense, easily-processed fuel product, is necessary to convert sugarcane into a bioenergy crop as there are existing markets for sugar that are currently more valuable than fuel. These three traits can be stacked together through traditional breeding, and is likely necessary to generate a single line that accumulates the targeted 20% TAG by dry weight and has a yield of 30 tons per hectare in the U.S.—the levels necessary to meet the program goal.

## PATHWAY TO ECONOMIC IMPACT

Illinois modeled the economic impact of producing biofuel from cane that accumulates various levels of TAG compared to conventional sugarcane in Brazil, and current biofuel crops in the U.S.: corn (ethanol) and soy (biodiesel). Oil could be extracted from the Illinois team's oilcane using existing crushing technologies for sugar extraction from cane. Based on current lipid processing technologies, the TAG from oilcane could be converted into biodiesel more cheaply than from a soy feedstock, and the remaining sugar in the cane could be converted into ethanol at a comparable cost to corn (Figure 4). At a level of just 2% TAG, oilcane would yield more biodiesel than soy on a per acre basis because of the high productivity of sugarcane. Based on metabolic modeling, Illinois expects to be able to reach 20% TAG in cane. Illinois has reached out to a number of industry partners in the fuel and chemicals sectors to incorporate the cane-derived TAG, which will be significantly cheaper than current sources such as soy, into existing biodiesel processes. Initial

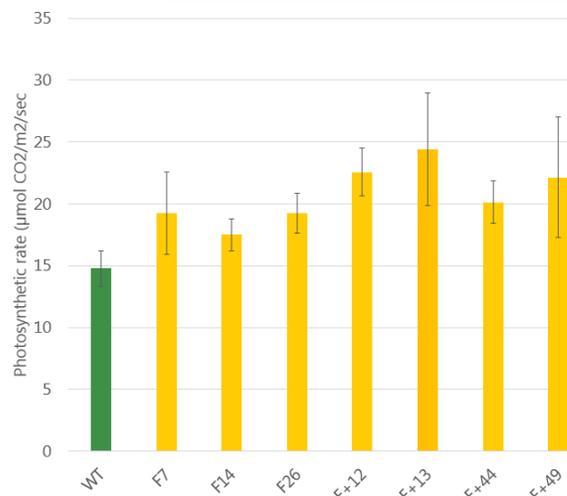


Figure 2: Light saturated photosynthetic rate (µmol CO<sub>2</sub>/m<sup>2</sup>/sec) in wild type and transgenic sugarcane.

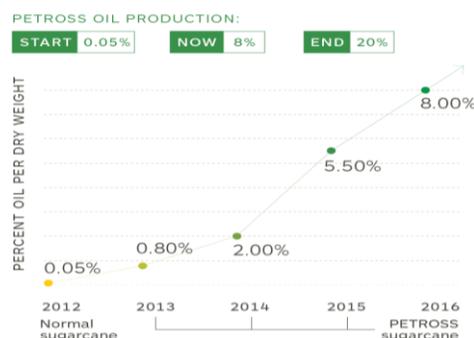


Figure 3: Increasing TAG content in transgenic sugarcane.

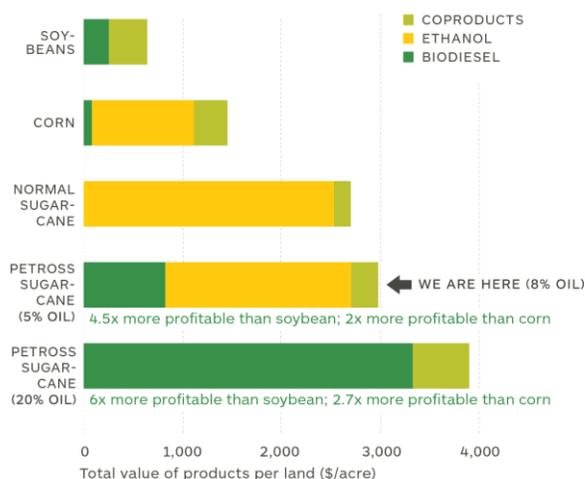


Figure 4: Value from soybean, corn, normal sugarcane, and oilcane.

interest for oilcane has come from Brazil because of its existing large-scale sugarcane acreage and mature biorefining infrastructure, and a group there is working towards field testing the Illinois oilcane in Brazil.

Illinois' photosynthesis traits have the potential to generally increase productivity in both fuel and food crops, and Illinois has received a \$25M grant from the Bill and Melinda Gates Foundation to utilize these traits in food crops. To move the most promising traits demonstrated in the PETRO project towards a first market, the Illinois team has partnered with Syngenta to validate the performance of Illinois' transgenic sugarcane in Syngenta's phenotyping facilities. If successful, Syngenta would license the traits and incorporate them into its commercial maize and sugarcane varieties for large-scale deployment.

## LONG-TERM IMPACTS

The long-term outcomes of this project would be the combination of the three promising traits that were demonstrated. If that can be accomplished, it could yield a new biodiesel crop feedstock with a range as far north as Arkansas, that at the target level of 20% TAG, would deliver 17 times the oil yield per acre as soybean, reducing the land dedicated to growing bioenergy crops instead of food.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of January 2017, the Illinois project generated three invention disclosures, one patent application, with one patent issued by the U.S. Patent and Trademark Office:

### Patent:

Long, S.P., Singh, V. and Huang, H. 2014. Separation process of oil and sugars from biomass. US Patent No. 9,394,503

The Illinois team has also published the scientific underpinnings of the technology in the open literature. The publications are provided below:

### Publications:

- Y. Wang, S.P. Long, X.G. Zhu (2014) Elements Required for an Efficient NADP-Malic Enzyme Type C4 Photosynthesis. *Plant Physiology* 164: 2231-2246
- K. Glowacka, S. Adhikari, J. Peng, J. Gifford, J.A. Juvik, S.P. Long, E.J. Sacks (2014) Variation in chilling tolerance for photosynthesis and leaf extension growth among genotypes related to the C4 grass *Miscanthus x giganteus*. *Journal of Experimental Botany*, doi: 10.1093/jxb/eru287
- D. Coursolle, J. Lian, J. Shanklin, H. Zhao (2015) Production of long chain alcohols and alkanes upon coexpression of an acyl-ACP reductase and aldehyde-deformylating oxygenase with a bacterial type-I fatty acid synthase in *E. coli*. *Mol. Biosyst.*, 2015, 9, 2464
- K. Glowacka, A. Ahmed, S. Sharma, T. Abbott, J. Comstock, S. Long, E. Sacks (2015) Can chilling tolerance of C4 photosynthesis in *Miscanthus* be transferred to sugarcane? *Global Change Biology Bioenergy*. DOI: 10.1111/gcbb.12283
- H. Huang, S.P. Long, V. Singh (2016) Techno-economic analysis of biodiesel and ethanol co-production from lipid-producing sugarcane. *Biofuels, Bioproducts and Biorefining*. DOI: 10.1002/bbb.1640
- H. Huang, S.P. Long, T.E. Clemente, V. Singh (2016) Techno-economic analysis of biodiesel and ethanol production from lipid-producing sugarcane and sweet sorghum. *Industrial Biotechnology*. DOI: 10.10889/ind.2016.0013
- J. Zale, J. Hyeong Jung, J. Yoon Kim, B. Pathak, R. Karan, X. Chen, H. Wu, H. Lui, J. Candreve, Z. Zhai, J. Shanklin, F. Altpeter (2015) Metabolic engineering of sugarcane to accumulate energy-dense triacylglycerols in vegetative biomass. *Plant Biotechnology Journal*. DOI: 10.1111/pbi.12411

# ENGINEERING THE OPTIMIZED BIOFUEL CROP

Updated: January 30, 2017

**PROJECT TITLE:** Engineering Enzymes in Energy Crops

**PROGRAM:** OPEN 2009

**AWARD:** \$3,914,527

**PROJECT TEAM:** Agrivida (Lead), University of Illinois at Urbana-Champaign

**PROJECT TERM:** January 2010 – March 2015

**PRINCIPAL INVESTIGATOR (PI):** Michael Raab

## TECHNICAL CHALLENGE

Biofuels offer alternative approaches to transportation fuels that support U.S. energy security, reduce dependence on energy imports, and can reduce net greenhouse gas (GHG) emissions dramatically. Domestically produced biofuels must address challenges in the sustainable production of bio-energy crops, as well as be cost-effective. Sustainability requires crops with high yields per land area, the ability to use land that is less useful for food crops, and reduced agronomic inputs (e.g. water, fertilizer, etc.). One approach to achieving this goal is to use cellulosic biomass, the stems and leaves of plants, as a feedstock for biofuels. However, cellulose is much more difficult to chemically process into biofuel compared to corn grain, and this challenge needs to be addressed to decrease the capital and operating costs of cellulosic biorefineries.

## TECHNICAL OPPORTUNITY

Advances in computational biology and structural biology have allowed researchers to rationally design enzymes with specific properties to optimize them for applications such as biomass deconstruction and fermentation. These technologies are allowing researchers to incorporate engineered enzymes into plants to produce enhanced bioenergy crops. Switchgrass, *Panicum virgatum*, is grass native to the United States (Figure 1) and was identified by the Department of Energy as one of the high priority crops for development as a dedicated bioenergy crop. Switchgrass is capable of high biomass yields with low levels of agronomic input, and because it is a perennial crop with a deep root system, it can effectively sequester carbon below ground. Lastly, the efficiency of genetic transformation for switchgrass has improved significantly, allowing researchers to routinely engineer desired traits into the plant.

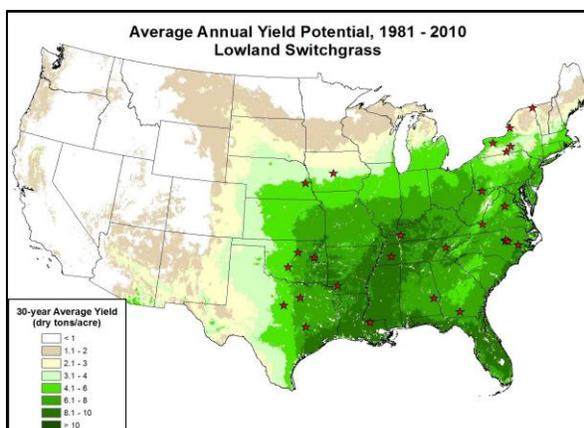


Figure 1: Potential yield mapping of switchgrass, as determined by the PRISM Climate Group. ([energy.gov/sites/prod/files/2014/11/f19/daly\\_biomass\\_2014.pdf](http://energy.gov/sites/prod/files/2014/11/f19/daly_biomass_2014.pdf))

## INNOVATION DEMONSTRATION

Agrivida's goal was to develop plant varieties that would be better feedstocks for cellulosic biofuels. Prior to the ARPA-E award, enzymes had been isolated from microbes that naturally degrade the cell walls in plant biomass into fermentable sugars, but these enzymes are costly to produce. Agrivida proposed to engineer plants so they directly produce these cell wall degrading (CWD) enzymes *in planta*, significantly decreasing the cost of enzyme production and improving their efficiency by placing the CWD enzymes next to the plant cell wall. The goal was to deliver switchgrass varieties expressing CWD enzymes and demonstrate how this biomass can be hydrolyzed with less severe pretreatment conditions. To achieve the project goals, Agrivida first had to optimize the enzymes for performance *in vitro*, and then demonstrate the transgenic switchgrass lines had improved processing.

Agrivida optimized the CWD enzymes through protein engineering so that they would be inactive during the life of the plant, protecting the plant from being damaged by the CWD enzymes while it was growing. This was done by inserting a blocker (intein) into the enzyme. The intein would be deactivated by a high temperature (> 60°C) trigger after harvest, and yield a functional CWD enzyme. Agrivida tested 157 intein variants. The best blocker candidate reduced enzyme

activity 10-fold when present in the enzyme, but yielded almost 80% of the activity of the native protein after heat treatment (Figure 2). The most promising inteins were engineered into a variety of CWD enzymes and transformed into switchgrass and corn.

After promising results in greenhouse studies, Agrivida obtained an environmental release permit from the United States Department of Agriculture (USDA) Animal and Plant Health Inspection Service to perform a field trial with two varieties of intein-CWD containing switchgrass. The transgenic switchgrass with the CWD enzyme grew as well as the native Alamo control variety. Pilot scale processing at both Agrivida's laboratory and a collaborator at the University of Illinois demonstrated that with only 20% of the normal full enzyme cocktail, the two transgenic switchgrass lines achieved the theoretical glucose yields of 68-71%. This compared with 52% for the negative control Alamo switchgrass line, represented a 40% improvement in glucose yield over the control Alamo biomass (Figure 3).

The project demonstrated both Agrivida's intein technology to control activity of enzymes *in planta*, and the effectiveness of embedding these intein-CWD enzymes in the plant to reduce recalcitrance of plant biomass. By modeling the state-of-the-art cellulosic biorefining process in 2015, Agrivida estimated that ethanol produced from its intein-CWD switchgrass would cost approximately \$0.80 less per gallon from a conventional switchgrass feedstock, a reduction of 30% of the total cost.

### PATHWAY TO ECONOMIC IMPACT

In 2012, Agrivida established a Joint Development Agreement with POET Research, Inc., one of the world's largest ethanol producers. POET worked with Agrivida to utilize Agrivida's technology platforms with the goal of significantly reducing the capital and operating costs of commercial cellulosic ethanol production facilities. However, with low oil prices, the economics of cellulosic ethanol production have been too challenging for POET to deploy Agrivida's enhanced crop feedstocks at scale in its biorefineries.

Agrivida is therefore developing an alternative path to first market entry, by providing enzymes in grain that are routinely added to animal feed products to improve the digestibility or increase the nutritional content, and consequently reduce the energy impacts of food production. When applied externally to animal feed, cell wall hydrolyzing enzymes improve the conversion efficiency of the feed by animals, reducing the quantity of feed needed, along with the energy used to produce the crops for feed. Agrivida has performed animal feeding studies following the completion of its ARPA-E award. These studies indicated that Agrivida's *in planta* enzyme technologies provide value to feed, and Agrivida is targeting the commercial release of feed products in the next two years, including those incorporating intein variants based upon work under its ARPA-E award.

Since Agrivida received its ARPA-E award, it has closed four rounds of private funding, totaling \$61M, to further develop and commercialize its technologies for the fuel and feed markets.

### LONG-TERM IMPACTS

Agrivida's intein-CWD enzyme enhanced feedstocks have demonstrated their efficacy in easing the processing of cellulose post-harvesting, while still allowing healthy plant growth. Success in the first-market strategy outlined above is expected

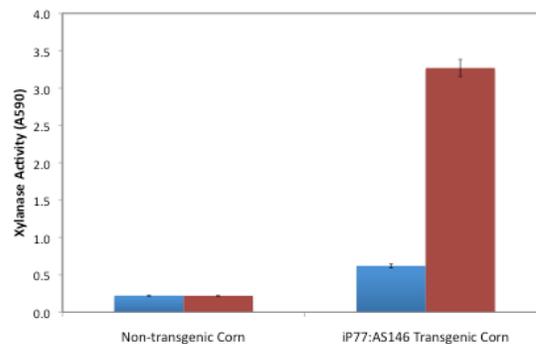


Figure 2: Level of enzymatic activity of control corn compared with transgenic intein-CWD corn. Samples were heated to 60°C to excise the intein and activate the enzyme.

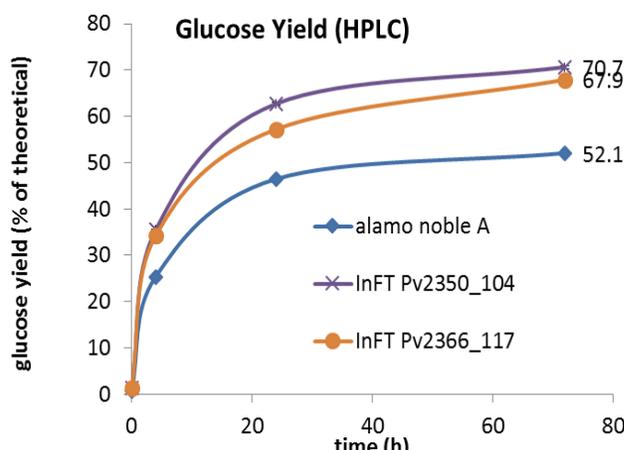


Figure 3: Level of glucose released using reduced enzyme loading from the biomass of two intein-CWD switchgrass compared to wild type Alamo. Percent glucose yield is calculated relative to the theoretical yield from the total cellulose in the plant.

to provide a foundation for future commercialization efforts in advanced biofuels and bio-based products. Agrivida's enhanced crops have been field tested, and its biomass demonstrated at the pilot scale. When the economics of cellulosic biofuel production become more favorable, Agrivida's feedstocks will be ready for scale up and commercial deployment. Furthermore, Agrivida's enhanced crops could become a significant feedstock for animal feed and their improved efficiency as feed could both reduce the energy inputs in meat production and the acreage needed to grow the feed.

## **INTELLECTUAL PROPERTY**

As of December 2016, the Agrivida team has generated four invention disclosures, three patent applications with the U.S. Patent and Trademark Office (PTO) and two patents:

AGRPT010.2WO, "*Intein-modified enzymes, their production and industrial applications*". U.S. Patent No. 9,464,333.

AGRPT015.1WO, "*Consolidated Pretreatment and Hydrolysis of Plant Biomass Expressing Cell Wall Degrading Enzymes*". U.S. Patent No. 9,249,474.

# LIQUID TRANSPORTATION FUEL FROM ELECTRICITY AND CO<sub>2</sub>

Updated: January 27, 2017

<b>PROJECT TITLE:</b> Bioprocess and Microbe Engineering for Total Carbon Utilization in Biofuel Production
<b>PROGRAM:</b> Electrofuels
<b>AWARD:</b> \$4,400,000
<b>PROJECT TEAM:</b> Massachusetts Institute of Technology (Lead), University of Delaware, & Harvard University
<b>PROJECT TERM:</b> July 2010 – March 2014
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Gregory Stephanopoulos

## TECHNICAL CHALLENGE

Biofuels have lower net carbon dioxide (CO<sub>2</sub>) emissions than traditional fuels, because they are derived from plants, which use CO<sub>2</sub> from the air to build their biomass. However, photosynthesis, the molecular process by which plants “fix” CO<sub>2</sub>, is very inefficient from an energy conversion perspective, converting only 2-4% of incident solar radiation into stored chemical energy in the form of C-C and C-H bonds.<sup>1</sup> Due to this inherent constraint, traditional biofuels require large land areas to produce the appreciable quantities of biomass required as a feedstock for production. The limitations of traditional biofuel approaches warrant innovation in the area of non-photosynthetic autotrophic production of biomass with the goal of infrastructure-compatible, energy-dense liquid fuels.

## TECHNICAL OPPORTUNITY

An alternative bioprocess for “fixing” CO<sub>2</sub> is through microorganisms termed chemoautotrophs that are capable of deriving energy not from the sun or from consuming sugar, but rather from inorganic energy sources such as hydrogen (H<sub>2</sub>) or carbon monoxide (CO). Some chemoautotrophs are even capable of directly accepting electrons from an electrode to power CO<sub>2</sub> conversion to fuel and chemical molecules. However, historically, these organisms have not been evaluated or applied to producing liquid fuels for transportation. Recent advances in synthetic biology and metabolic engineering, along with the availability of genetic sequence information have demonstrated significant potential to modify microbiological metabolic pathways to produce non-native chemicals and fuels in chemoautotrophic microbes.

## INNOVATION DEMONSTRATION

The Massachusetts Institute of Technology (MIT) led team’s goal was to produce an infrastructure compatible fuel starting from CO<sub>2</sub> and H<sub>2</sub>, or CO, instead of sugars. The target fuel was energy-dense lipids called triacylglycerides (TAGs). The overall strategy involved an integrated two-stage reactor system for 1) fixing CO<sub>2</sub> with H<sub>2</sub>/CO with an “acetogenic” microorganism to produce acetate and 2) feeding acetate to an “oleaginous” yeast capable of achieving very high lipid yields, productivities, and titers (Figure 1).

The first technical challenge in this project was to develop a chemoautotroph capable of producing acetate from CO<sub>2</sub> and H<sub>2</sub> at high productivity and yield. The major challenge was that engineering chemoautotrophs was uncharted. University of Delaware (UD) leveraged whole genome sequencing, to engineer *C. ljungdahliae* to produce and secrete acetate. The team developed a genetic system to stably delete or “knock-out” specific genes in a targeted manner. Specifically, UD

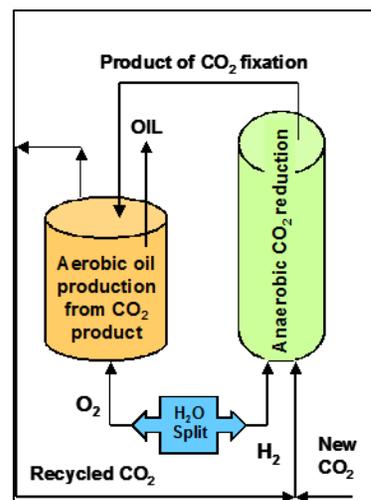


Figure 1: Two-stage reactor system, with chemoautotrophic reduction of CO<sub>2</sub> to create a product (acetate) that becomes the input to fermentation process for production of natural oils (TAGs).

<sup>1</sup> Borak, B., Ort, D.R., Burbaum, J.J. Energy and carbon accounting to compare bioenergy crops. Current Opinions Biotechnology 2013 Jun;24(3):369-75

researchers demonstrated controlled genetic disruption that was stable on the chromosome for over 80 generations. This technique enabled targeting for deletion specific transcription factors (e.g sigK) postulated to be essential for sporulation. Clostridia produce acetate in order to generate ATP to power cell growth. However, when preparing for sporulation, Clostridia will utilize acetate and generate acetone. The team hypothesized that the sigK knock-out would halt sporulation and acetate utilization. The UD team demonstrated that their hypothesis was correct. The team observed that, acetate utilization was curtailed in the sigK knock-out, resulting in an increase in acetate production relative to wild type by 30%. The technique was a first for demonstrating how new genetic tools could be applied to Clostridia for increasing acetate production.

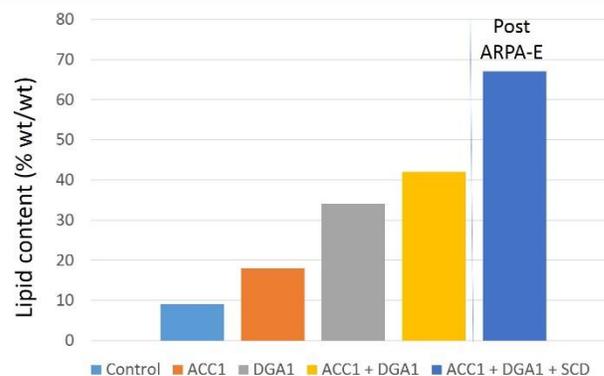


Figure 2: Overexpression of key enzymes identified by MIT significantly increases lipid content.

The second technical challenge was to achieve very high lipid yields through an oleaginous yeast using acetate as the feedstock. The team had prior art on engineering the yeast *Y. lipolytica* for increased lipid production.<sup>2</sup> The challenge for the MIT team was to significantly increase the amount of lipid on a weight per weight basis to > 50% - a range that had not been achieved by oleaginous yeast or microalgae grown under phototrophic conditions. The MIT team devised a strategy to create high carbon flux to TAGs through the overexpression of the enzymes acetyl-CoA carboxylase (ACC) and diacylglycerol (DAG) in the yeast, and demonstrated a 5-fold increased lipid content (Figure 2). The team created significant improvements in oil production from sugar achieving titers of 20-30 g/L at lipid yields of ≥60% of theoretical maximum and productivities of 0.6-1.0 g/L/h by the end of the ARPA-E award period.

The MIT team leveraged the technical accomplishments achieved under the ARPA-E award to demonstrate integration of chemoautotrophic production of acetate followed by heterotrophic lipid production. Integration of the two technologies required development of hollow fiber membrane and cell recycle unit operations to achieve high biocatalyst loading and product titer. The first stage is an anaerobic bioreactor, in which H<sub>2</sub> reduces CO<sub>2</sub> to 30 g/L acetate, followed by the second stage where acetate is utilized for TAG production. In 2016, after the conclusion of the ARPA-E award, the team published continued research into the integrated, continuous two-stage reactor system and demonstrated production of natural oils from a mixture of gases of CO<sub>2</sub> and CO or H<sub>2</sub>. The system produced 18 g/L of C16-C18 TAGs at a productivity of 0.2 g/L/hr and final lipid content of 36% in its integrated form of the two-stage bioreactor system (Figure 3).<sup>3</sup>

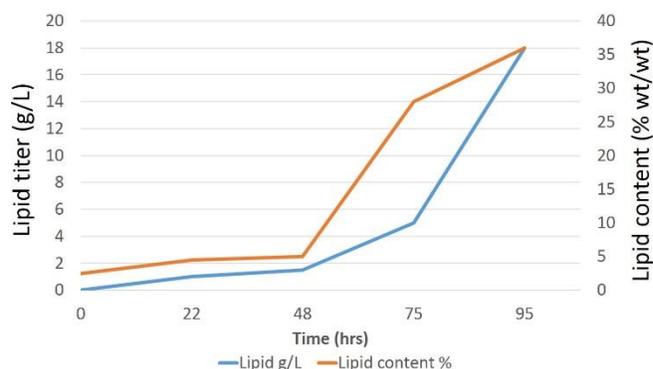


Figure 3: Lipid titer and biomass production in an integrated process.

## PATHWAY TO ECONOMIC IMPACT

The project demonstrated the feasibility of modifying chemoautotrophs for bioengineering applications, with potential applications in fermentation of syngas. It also showed that a two stage chemoautotroph-heterotroph bioprocess can produce lipid yields comparable to yields achieved using microalgae fed with sugar, and significantly higher than

<sup>2</sup> Syed Hussain Imam Abidi and Gregory Stephanopoulos, "Microbial engineering for the production of fatty acids and fatty acid derivatives," (Filed: 3/2/2010, ref. Number: M0656.70204US00).

<sup>3</sup> Hu, P. et al. "Integrated bioprocess for conversion of gaseous substrates to liquids" *Proceedings of the National Academy of Sciences* 2016 113 (14), 3773-3778.

microalgae grown under phototrophic (no sugar) conditions. Much of this work was transferred to the public domain in the form of reports and publications, as reflected in the Intellectual Property and Publications section below.

Through licensing, the for-profit biotechnology company Novogy has acquired the use of genetically engineered yeast biocatalysts developed at MIT for the production of lipids. Work at both MIT and Novogy continues and improvements have been validated. Currently, the team has increased lipid titers using glucose as the feedstock to 100 g/L at yields of 0.28g/g, values in scope of commercial potential in anticipated first markets such as animal feeds.

MIT continues to develop *Y. lipolytica* as a biocatalyst for industrially-relevant bioprocessing. Post ARPA-E, MIT identified the enzyme delta-9-stearoyl-CoA desaturase (SCD) as a rate limiting step in the lipid biosynthesis pathway and as a new target for overexpression. When combined with ACC and DAG, SCD overexpression further increased lipid content to nearly 70% wt/wt. *Y. lipolytica* can also grow on acetate and other volatile fatty acids, products of anaerobic digestion of various wastes. Using cell recycle and metabolism-based controls of feed, lipid titers in excess of 120g/L have been achieved on acetate at productivities in the range of 1g/L/hr.

The MIT-led project significantly advanced the technologies needed for commercialization of biofuel production based on chemo-autotrophic organisms. Continuing challenges for commercialization are the need for the supply of a low-cost reducing agent such as of H<sub>2</sub> and further technology advancement to ensure that the integrated system depicted in Figure 1 achieves the performance that has been demonstrated for each individual unit.

## LONG-TERM IMPACTS

The work on chemoautotrophs such as *C. ljundahlii*, though still in early-state development, provides a pathway to bypass photosynthesis for CO<sub>2</sub> utilization. The ability to process CO<sub>2</sub> through bioengineering approaches that do not require light input provides a future option to complement traditional agricultural production of biomass, and as a potential pathway to carbon capture and utilization.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of January 2017, the MIT team's project has resulted in two invention disclosures, two U.S. PTO patent applications, and two U.S. PTO issued patents:

### Patents:

Methods for Microbial Oil Overproduction from Cellulosic Materials. US Patent 9096876. (2015) Washington, DC: U.S. Patent and Trademark Office.

Methods for Microbial Oil Overproduction via Amplification of the Biosynthetic and Sequestration Pathways Individually or in Combination. US Patent 8951776. (2015) Washington, DC: U.S. Patent and Trademark Office.

The MIT and UD team has also published the scientific underpinnings of this technology extensively in the open literature. A list of publications is provided below:

### Publications:

"Integrated bioprocess for conversion of gaseous substrates to liquids," Hu, P; Chakraborty, S; Kumar, A; Woolston, B; Liu, HJ; Emerson, D; Stephanopoulos, G, Proceedings of the National Academy of Sciences of The United States Of America, Vol. 113, Issue 14, Pg. 3773-3778, 2016. (4 times cited)

"Sigma(K) of *Clostridium acetobutylicum* Is the First Known Sporulation-Specific Sigma Factor with Two Developmentally Separated Roles, One Early and One Late in Sporulation," Al-Hinai, MA; Jones, SW; Papoutsakis, ET, Journal Of Bacteriology, Vol. 196, Issue 2, Pg. 287-299, 2014. (15 times cited)

"Anaerobic CO<sub>2</sub> fixation by the acetogenic bacterium *Moorella thermoacetica*," Hu, P; Rismani-Yazdi, H; Stephanopoulos, G, Aiche Journal, Vol. 59, Issue 9, Pg. 3176-3183, 2013. (9 times cited)

"Engineering *E. coli* for caffeic acid biosynthesis from renewable sugars," Zhang, HR; Stephanopoulos, G, Applied Microbiology and Biotechnology, Vol. 97, Issue 8, Pg. 3333-3341, 2013. (23 times cited)

"Stoichiometric and energetic analyses of non-photosynthetic CO<sub>2</sub>-fixation pathways to support synthetic biology strategies for production of fuels and chemicals," Fast, AG; Papoutsakis, ET, Current Opinion in Chemical Engineering, Vol. 1, Issue 4, Pg. 380-395, 2012. (38 times cited)

Tracy, BP, Jones, SW, Fast, AG, Indurthi, DC, and Papoutsakis, ET. 2012. Clostridia: the importance of their exceptional substrate and metabolite diversity for biofuel and biorefinery applications. Curr. Opin. Biotechnol. 23: 364-381 (DOI: 10.1016/j.copbio.2011.10.008). (133 times cited)

# CONVERTING CARBON DIOXIDE INTO FUEL

Updated: September 23, 2016

**PROJECT TITLE:** Energy Efficient Electrochemical Conversion of Carbon Dioxide into Useful Products

**PROGRAM:** OPEN 2012

**AWARD:** \$4,877,240

**PROJECT TEAM:** Dioxide Materials (Lead), 3M

**PROJECT TERM:** February 2013 – January 2017

**PRINCIPAL INVESTIGATOR (PI):** Dr. Rich Masel

## TECHNICAL CHALLENGE

The United States releases a large amount of carbon dioxide (CO<sub>2</sub>) into the atmosphere each year—about 5.4 billion tons annually from all sectors. The research community has made progress in methods for carbon capture, but an economically attractive use for the CO<sub>2</sub> is needed to lower the costs of reducing carbon emissions via capture. One possibility is to convert CO<sub>2</sub> to useful chemical products. However, CO<sub>2</sub> is chemically unreactive, so its conversion to the reactive precursor, carbon monoxide (CO), or other chemicals is tremendously difficult to do cost-effectively. Electrochemical approaches to this problem have been hindered because of large activation barriers (over-potentials) that create a large energy requirement for conversion.

## TECHNICAL OPPORTUNITY

The electrochemical conversion of CO<sub>2</sub> into useful products has been studied for decades, but until 2011, all of the existing processes suffered from the need for large over-potentials, and/or limited selectivity to desired products. In 2011, researchers from Dioxide Materials reported success with using an ionic-liquid-mediated process that stabilizes the high-energy anionic intermediation in the CO<sub>2</sub> to CO conversion, thus significantly lowering the over-potential as illustrated in Figure 1.<sup>4</sup> CO is a precursor to a large set of chemical processes used to create hydrocarbon products (e.g., in a Fischer-Tropsch plant or bioreactor), so an improved pathway to CO production from CO<sub>2</sub> opens new opportunities for CO<sub>2</sub> utilization.

## INNOVATION DEMONSTRATION

The major requirements for designing an electrochemical cell that produces CO economically are: 1) a low over-potential reaction, which selectively converts CO<sub>2</sub> to CO; 2) a high enough current density to minimize the size of the cell need for high rates of chemical conversion; 3) a long life time; 4) the potential to scale up the design to show that the chemistry works at industrial scales. The project started with Dioxide Materials' ionic liquid containing membrane electrode assembly (MEA, Figure 2), which showed low over-potential and 99% selectivity, but low turn-over rate. Over the course of the four-year project, the Dioxide Materials team increased the reaction rate, as demonstrated by increasing current per unit area over

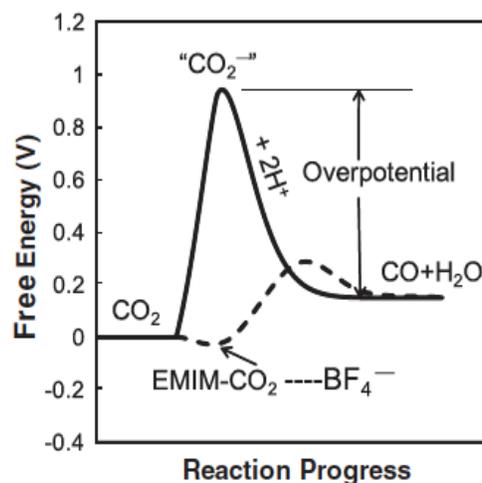


Figure 1: Schematic of reduced over-potential by stabilization of the anionic intermediate. Solid line: reaction pathway in water solvent; dashed line: reaction pathway in ionic liquid.

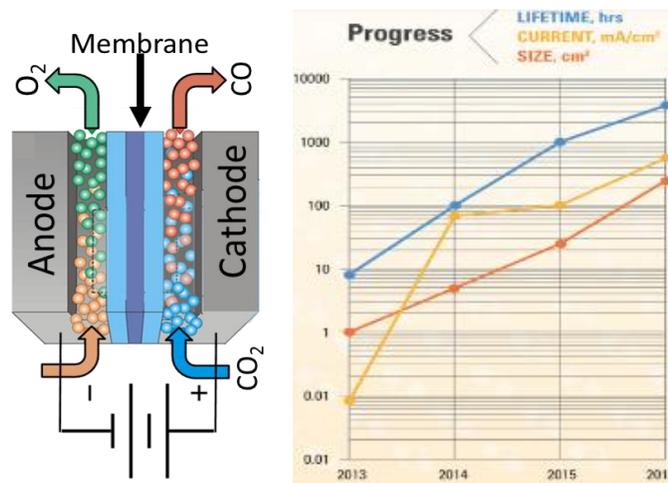


Figure 2: Device schematic and improvement of key metrics.

<sup>4</sup> Rosen, B.A., et al., Ionic Liquid Mediated Selective Conversion of CO<sub>2</sub> to CO at Low Overpotentials. *Science*, 2011. 334 p. 643-644.

4000 times from 0.08 mA/cm<sup>2</sup> to 400 mA/cm<sup>2</sup>, and increased the lifetime over 500 times, from 8 hours to 4,500 hours by systematically tuning the cell design and ionic liquid composition.

In parallel, 3M helped in scaling up the components of the MEA towards a roll-to-roll process, while maintaining cell performance and evaluating alternate designs. This aided in addressing the final challenge of scaling up the device size from 1 cm<sup>2</sup> to 250 cm<sup>2</sup>. Through this effort, the team has increased the total CO production volumes by a factor of one million. The team is currently demonstrating manufacturing the membrane in a roll-to-roll process in order to prepare materials for sales and build a pilot-scale facility. The team's techno-economic analysis has identified four entry-point commodity chemical markets for the Dioxide Materials CO<sub>2</sub> electrolysis process: CO to 1) polycarbonate, 2) formic acid, 3) acrylic acid, and 4) renewable fuels. The next stage is to build larger cells and stacks for a pilot electrolyzer.

## PATHWAY TO ECONOMIC IMPACT

Dioxide Materials' development plan is first entering small, addressable markets for their membranes to drive down costs and improve their manufacturing process. Figure 3 outlines a market strategy that initially targets CO<sub>2</sub> sensors through a technology licensing agreement. In parallel with the sensor sales, the company is pursuing direct sales of the proprietary anion exchange fuel cell membrane. By making these membranes available to academic and industrial researchers, Dioxide gains both a beachhead revenue stream for the company and direct feedback from customers for sustained improvement and optimization of the membrane and the scale-up of the manufacturing.

The membrane manufacturing process development is being supported by 3M Corporation, which has been a cost share partner throughout the ARPA-E project and is a world-leader in the scale up of electrochemical assemblies and fuel cells.

Beyond the beachhead markets, Dioxide Materials plans to develop commercial electrolyzers that can be used to produce the CO precursor for renewable fuels and chemicals, and license them world-wide in partnership with 3M. This will first be done through pilot scale electrolyzer projects. The pilot is designed, and the Dioxide Materials/3M team has demonstrated production of the needed membranes. Dioxide Materials has ongoing commercial discussions about applications in CO<sub>2</sub> waste stream utilization with a range of industrial chemical producers, including Modac, Linde, and Siemens.

## LONG-TERM IMPACTS

Dioxide Materials' CO<sub>2</sub> electrolyzer is a significant advance toward the goal of CO<sub>2</sub> utilization as part of worldwide CO<sub>2</sub> mitigation efforts. The targeted long-term impact is commercial technology that allows chemical manufacturers to make fuels and chemicals at a competitive cost while simultaneously providing a use for CO<sub>2</sub> that is captured to reduce CO<sub>2</sub> emissions into the atmosphere. Fuel production from CO<sub>2</sub> is the market with the largest potential for reducing net CO<sub>2</sub> emissions. Individually, chemicals have smaller production amounts (e.g. total U.S. market for acrylic acid is 5.2 Mton), but larger profit margins that provide the opportunity to enter manufacturing and drive down costs.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of August 2016, the project has generated six invention disclosures to ARPA-E, six U.S. Patent and Trademark Office (PTO) patent applications and one issued patent.

### Patent:

"Ion-conducting membranes" (2016) U.S. Patent No. 9,370,773 B2. Washington, DC: U.S. Patent and Trademark Office

The team has also published the scientific underpinnings of this technology in the open literature. A list of publications is provided below:

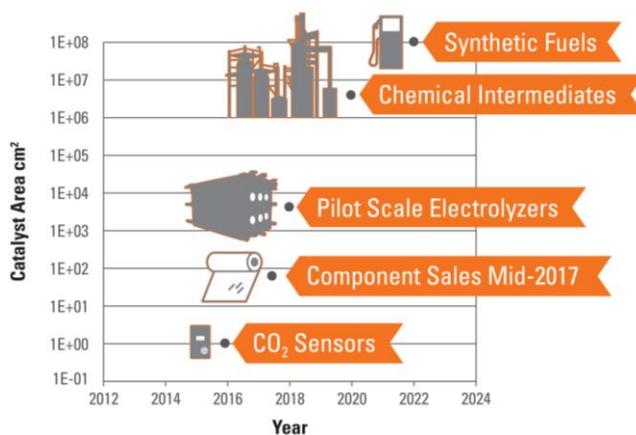


Figure 3: Markets relative to scale of device.

### Publications:

Masel, R., R. Ni, Z. Liu, Q. Chen, R. Kutz, L. Nereng, D. Lutz, and K. Lewinski, Unlocking the Potential of CO<sub>2</sub> Conversion to Fuels and Chemicals as an Economically Viable Route to CCR. *Energy Procedia*, 2014. 63: p. 7959-7962.

Masel, R. and Liu, Z. and Zhao, D. and Chen, Q. and Lutz, D. and Nereng, L, CO<sub>2</sub> conversion to chemicals with emphasis on using renewable energy/resources to drive the conversion, *RSC Green Chemistry*, 43(2016) 215-257.

Verma, S., X. Lu, P.J.A. Kenis, S. Ma, and R.I. Masel, The Effect of Electrolyte Composition on the Electroreduction of CO<sub>2</sub> to CO on Ag Based Gas Diffusion Electrodes. *Phys Chem Phys*, 2016. 18: p. 7075-84.

Zengcai Liu, Richard I. Masel, Qingmei Chen, Robert Kutz, Hongzhou Yang, Krzysztof Lewinski, Tyler S. Matthews, Marina Kaplun, Sean Luopa, Dale R. Lutz, Electrochemical Generation of Syngas from Water and Carbon Dioxide at Industrially Important Rates, *J. CO<sub>2</sub> Utilization*, 2016, 15 p 50-56.

# CHEAPER, FASTER WASTE-GAS FERMENTERS FOR FUELS AND CHEMICALS

Updated: October 18, 2016

**PROJECT TITLE:** Process Intensification through Innovative Bioreactor Designs

**PROGRAM:** Reducing Emissions using Methanotrophic Organisms for Transportation Energy (REMOTE)

**AWARD:** \$4,000,000

**PROJECT TEAM:** LanzaTech (Lead); City University of New York; Louisiana State University; University of California, San Diego; San Diego State University; Michigan Technological University

**PROJECT TERM:** January 2014 – January 2017

**PRINCIPAL INVESTIGATOR (PI):** Dr. Derek Griffin

## TECHNICAL CHALLENGE

Gas-to-liquid processes enable monetization of gas resources through production of fuels and chemicals. Microorganisms have been demonstrated to effectively convert a variety of gas streams to fuels and other products via gas fermentation, in which the microbes consume gases for carbon and energy, rather than sugars as in traditional fermentation. A key technical challenge for gas fermentation, especially at small scales, is designing a cost effective and energy efficient fermenter (bioreactor) that enables very high rates of gas transfer into the fermentation liquid. Process intensification through development of novel and highly efficient bioreactors will have a broad impact by enabling economic production of fuels from multiple gas streams that would otherwise be emitted, flared or combusted for power generation, generating carbon dioxide (CO<sub>2</sub>). These gas streams contain carbon monoxide (CO), CO<sub>2</sub>, hydrogen (H<sub>2</sub>), and methane (CH<sub>4</sub>), and can come from:

- Waste industrial gases that have already served a primary purpose
- Biogas from landfills, anaerobic digestion and other sources
- Stranded and associated natural gas

Only a small number of these gas sources are of sufficient scale to enable competitive fuel production economics today. Production of liquid fuels from the numerous smaller gas sources that are not yet economical may become cost effective with increased bioreactor efficiency.

## TECHNICAL OPPORTUNITY

Enhancing gas-to-liquid mass transfer has been a long-standing challenge in the bioprocessing industry and a wide range of fermenter designs have been tested to address this problem. While high gas transfer rates can be achieved, it is typically at the cost of high energy input. A key to improvement is to maximize the area of the interface between the gas and liquid phases. Advances in computational fluid dynamics modelling and innovative experimental tools to assess experimental performance now make it possible to design and construct a bioreactor that uses this approach to significantly reduce capital and operating costs.

## INNOVATION DEMONSTRATION

The primary objective of this project has been to develop a new type of bioreactor which maximizes gas mass transfer by creating a large gas surface area per unit volume, and maintains that high surface area throughout large parts of the total reactor volume, giving the gas enough residence time to be fully utilized. To address this challenge, the LanzaTech team designed and built a new type of microbubble reactor, which combines a novel device for microbubble formation with a reactor geometry and liquid circulation approach which has dramatically increased gas mass transfer coefficients by nearly one order of magnitude above that in state of the art gas liquid bioreactors. Using computational fluid dynamics (CFD) modeling, the team was able to optimize the



**Figure 1:** Picture of test reactor showing very fine bubble distribution.

geometry of the microbubble generator to reduce energy losses. The project team also designed and deployed special high-speed cameras to visualize bubble size and bubble distribution in the reactor, which was necessary to validate and refine the CFD model used to optimize the fluid flow in the reactor. The new design, which has been demonstrated at a 200L scale, can double the amount of gas transferred per unit of energy input compared to even the next best airlift reactor design.

To test the new reactor design with a representative gas-consuming microorganism, LanzaTech used its well established CO fermenting organisms. Using the new reactor design they were able to increase the gas uptake rate by the microorganisms by 50% per unit reactor volume. This higher gas uptake rate also resulted in doubling of the biomass productivity in the new reactor vs. their best reference system. The experimental fermentation data also allowed the project team to further update the CFD model of the reactor to better reflect the conditions in a reactor containing real fermentation broth including microorganisms.

The practical results of this new design are the ability to reduce the required reactor volume by two thirds without having to increase the system pressure. This in turn lowers the energy requirement for gas compression, one of the main operating cost parameters in gas fermentation, by approximately 80%.

The team is currently working on further improving the reactor design based on fermentation data and will also test the system with methanotrophic microorganisms. A system energy audit will provide critical performance data that will inform techno-economic analysis (TEA) and life-cycle assessment (LCA) performance models, which will guide scale-up efforts.

## PATHWAY TO ECONOMIC IMPACT

LanzaTech's process intensification technology for the fermentation of gases has successfully advanced the state-of-the-art in mass transfer, such that mass transfer of the gases into solution now exceeds the current uptake abilities of the fermentation organisms. The engineering and accessory equipment sizing improvements result in an overall reduction in plant capex that the team's technoeconomic assessment indicates is sufficient to shift more projects into commercial viability.

The next step towards the commercial impact of this technology will be to integrate the new reactor into existing LanzaTech process designs by building and optimizing a demonstration plant at 1/10 scale (18-24 months) followed by construction and startup of the first commercial unit (additional 18-24 months). These first commercial units are expected to be commissioned as part of the roll out of LanzaTech's existing CO and CO<sub>2</sub> fermentation processes used to recycle waste gases from steel mills and other industrial facilities. The first publicly reported project with a conventional reactor is under construction now alongside the steel maker ArcelorMittal that will harvest waste gases from a steel plant to produce 64,000 tons of ethanol per year.

The team's assessment indicates that the improved bioreactor offers the potential for capital and operating cost reductions over the current state-of-the-art. This cost advantage provides an opening for bio-recycling of waste gases to competitively target the 25 separate chemical markets, including ethanol, for which LanzaTech is engineering and optimizing their industrial waste gas organisms.

## LONG-TERM IMPACTS

As an example of the potential scale of impact, about 60% of the worldwide production of 'crude steel' by the basic oxygen furnace (BOF) process is market-addressable for capture of BOF gas. If this is all converted to ethanol, this has the potential of producing 19 million tons (6.4 billion gallons) per annum. Given that LanzaTech ethanol reduces greenhouse gases (GHGs) emissions over conventional gasoline by 65% on average, producing 19 million tons of ethanol per year would bring a reduction of 31 million tons of CO<sub>2</sub>.

In addition to transportation fuels, early target markets for the recycled waste gas-to-products technology are styrene butadiene (\$13B/year), polybutadiene (\$8B/year), acrylonitrile butadiene (\$16B/year), and nylon 6,6 (\$7B/year). Finally, the fermentation technology may be applied to other waste gases including wellsite-flared natural gas. By bringing waste and underutilized carbon (CO, CO<sub>2</sub>, flared methane) back into the industrial cycle, LanzaTech estimates that the material impact is a reduction of hundreds of billions of gallons per year in oil-equivalent fossil energy consumption, with over 700 million tons of CO<sub>2</sub> emissions eliminated per each 100 billion gallons of fossil fuels not used.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of September 2016, the LanzaTech team has reported one invention and published the following articles regarding the scientific underpinnings of this technology:

*"Comparison of gas hold-up profiles in co-current, counter-current, and batch bubble column reactors measured using gamma densitometry and surface of revolution method,"* F. Hernandez-Alvarado, D. Kalaga, S. Banerjee, M. Kawaji. ASME 2016 Summer Heat Transfer Conference Proceedings, HTFEICNMM2016-1025, 2016.

*"Numerical and Experimental Analysis of Single Phase Jet Interactions,"* F. Hernandez-Alvarado, R. Samaroo, D. Kalaga, T. Lee, S. Banerjee, M. Kawaji. ASME 2016 Summer Heat Transfer Conference Proceedings, HTFEICNMM2016-1026, 2016.

*"Effect of surfactant addition on void fraction distributions measured by a wire mesh sensor,"* S. Kleinbart, F. Hernandez-Alvarado, D. Kalaga, D. Turney, J. Pulido, S. Banerjee, M. Kawaji. ASME 2016 Summer Heat Transfer Conference Proceedings, HTFEICNMM2016-1047, 2016.

# FLAMELESS COMBUSTION: CHEMICAL LOOPING ETHANE TO ETHYLENE

Updated: January 23, 2017

**PROJECT TITLE:** Electrogenerative System for Co-Production of Green Liquid Fuels and Electricity from Methane

**PROGRAM:** OPEN 2012

**AWARD:** \$4,665,228

**PROJECT TEAM:** EcoCatalytic (Formerly, Bio2Electric, LLC) (Lead), North Carolina State University, Particulate Solid Research Inc., KBR, Inc.

**PROJECT TERM:** February 2013 – July 2017

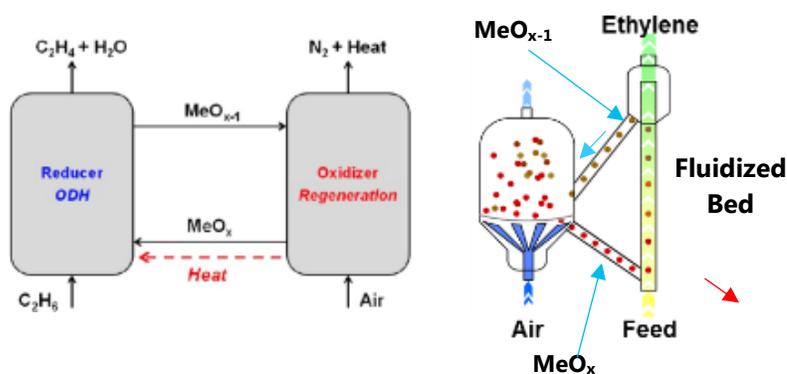
**PRINCIPAL INVESTIGATOR (PI):** John Sofranko

## TECHNICAL CHALLENGE

Ethylene is a major chemical feedstock, with 24 million metric tons produced domestically as of 2010<sup>5</sup>. In the U.S., ethylene is primarily produced in steam crackers from ethane, a byproduct of natural gas production. Domestic ethylene production consumes over 400 Trillion British Thermal Units (Tbtu) per year and releases over 30 million tons of carbon dioxide and harmful nitrogen oxides. One alternative to steam cracking of ethane is oxidative dehydrogenation (ODH), where ethane and oxygen react over a catalyst to form ethylene. ODH has a modest external heat requirement, and because air is excluded from the reactor, no nitrogen oxides are formed. However, supplying pure oxygen typically requires a cryogenic air separation unit, which negates the cost and energy savings. The highly volatile, capital intensive, commodity chemicals industry requires new technologies to be competitively priced as well as environmentally beneficial to enable adoption.

## TECHNICAL OPPORTUNITY

An alternative to providing pure gas-phase oxygen is to combine the catalyst with oxygen in a metal-oxide compound (MeO<sub>x</sub>). Circulating fluid bed chemical looping reactors use such oxygen transfer agents to promote chemical reactions, as illustrated in Figure 1. The oxygen transfer agent catalytically provides the oxygen to oxidize ethane to ethylene, producing water as the only major byproduct. The oxygen transfer agent then reacts with oxygen (regeneration) in a stream of air, at the same time producing heat to support the reduction process. By avoiding an air separation unit, these reactors are net exporters of energy in contrast to the energy intensive conventional processes. Chemical looping reactors have traditionally been used in combustion-related applications, and with innovation, chemical looping oxidative dehydrogenation offers an opportunity to reduce the energy emissions footprint of production of ethylene from ethane.



**Figure 1: Chemical looping oxidative dehydrogenation technology prevents air exposure for the reaction, ensures simultaneous engagement of the reactant with oxygen and the catalyst, and reduces energy use and emissions. A fluidized bed reactor design enables continuous processing.**

## INNOVATION DEMONSTRATION

The EcoCatalytic team's goal is to convert ethane to ethylene with reduced energy and emissions by way of chemical looping oxidation. This required developing an oxygen transfer agent that is chemically and physically robust to cycling between air

<sup>5</sup> Bandwidth Study on Energy Use and Potential Energy Saving Opportunities in U.S. Chemical Manufacturing, U.S.DOE Advanced Manufacturing Office, June 2015.

and feed reactors and that will facilitate ethylene production from ethane with high conversion and selectivity. They also needed to design a reactor system that balances the mass and heat flows for maximum efficiency.

The team adapted a metal-oxide catalyst to provide the properties needed to carry out the reaction in a fluidized bed configuration. This requires that the metal oxide material be fabricated into robust particles of similar size and strength to Fluid Catalytic Cracking (FCC) catalysts (70-100  $\mu\text{m}$  diameter). The development process involved adding different metal oxides to the mix of materials, and testing them for activity, selectivity, cyclability, and physical durability through experimentation and simulation. Cost has also been a crucial criterion in the selection process. The team developed a cyclable oxygen transfer agent that charges in air and reacts with ethane to produce 70% yield of useful products, of which ethylene is the primary output.

The team expended considerable effort in developing the reactor design, shown schematically in Figure 1. After extensive simulation of different designs, the team is now commissioning a 10 kW<sub>th</sub><sup>6</sup> chemical looping reactor that they will use to test their materials and reactor design. This laboratory-scale reactor, which will produce ethylene at a rate of up to 30 kg per day, is scheduled to be complete by June 2017. Their process models, validated by industrial partners and external consultants, indicate that their chemical looping oxidative dehydrogenation is projected to reduce total ethylene production costs by at least 20% and reduce carbon dioxide emissions, nitrogen oxide emissions, and production energy each by over 80%.

## PATHWAY TO ECONOMIC IMPACT

EcoCatalytic partnered with engineering, procurement, and construction company KBR to develop a techno-economic analysis of their technology and to validate estimates of energy use and emissions. Their analysis indicates that chemical looping oxidative dehydrogenation of ethane to ethylene has an improved emissions profile over the state of the art and an improved economic profile, with a total cost of production that is 20% less than traditional steam cracking. Thus, EcoCatalytic's technology has the potential to displace existing ethylene production, resulting in increased energy efficiency and reduced emissions.

Upon validating these models in their 10 kW reactor, EcoCatalytic will work with commercialization partners to validate their results at a larger pilot scale of 100 kW to 2 MW, equivalent to 0.5 to 10 metric tons of ethylene per day. To achieve this scale, the team is looking for opportunities in retrofitting existing reactors with an estimated initial capital investment of about \$5 million. The company is currently targeting business development for applications where reduced nitrogen oxide is a compelling value proposition, such as in the EPA non-attainment zones along the U.S. Gulf Coast.

## LONG-TERM IMPACTS

EcoCatalytic's technology is showing potential to lower the cost of ethane to ethylene production by 20%, thereby injecting competitive advantages into this industry that provides about 85,000 jobs nationwide<sup>7</sup>. As of 2010, the U.S. produces 24 million metric tons of ethylene per year<sup>5</sup>, constituting an output of \$30 billion in a global market worth over \$150 billion.<sup>8</sup>

Ethylene production in the U.S. consumes 400 TBtu of energy per year and releases 30 million tons of carbon dioxide into the atmosphere. Replacement of conventional ethylene production technology with chemical looping oxidative dehydrogenation has the potential to decrease energy consumption by over 300 TBtu per year and carbon dioxide emissions by over 25 million tons per year.

More broadly, the demonstration of a successful dehydrogenation process for ethane may also open development opportunities for similar improvements in other industrial chemical processes.

---

<sup>6</sup> Thermal, as opposed to electric.

<sup>7</sup> Estimated based on the total U.S. production volume and employment projections released by Louisiana Economic Development: [https://www.opportunitylouisiana.com/led-news/news-releases/news/2016/06/14/lotte-chemical-axiall-break-ground-on-\\$3-billion-complex-in-louisiana](https://www.opportunitylouisiana.com/led-news/news-releases/news/2016/06/14/lotte-chemical-axiall-break-ground-on-$3-billion-complex-in-louisiana)

<sup>8</sup> <http://mediatracking.com/npcapp/bounce.aspx/mynewsclips/30076/0/bXIOZXdzQ2xpcHMgUjINTIFVzZXI~/1193056782>

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of January 2017, the Bio2Electric team's project has generated three invention disclosures to ARPA-E and one U.S. Patent and Trademark Office (PTO) patent application. The team has also published the scientific underpinnings of this technology in the open literature. A list of publications is provided below:

Haribal, V. P., Neal, L. M., & Li, F. (2016). Oxidative dehydrogenation of ethane under a cyclic redox scheme—Process simulations and analysis. *Energy*. <http://dx.doi.org/10.1016/j.energy.2016.11.039>

Neal, L. M., Yusuf, S., Sofranko, J. A., & Li, F. (2016). Oxidative Dehydrogenation of Ethane: A Chemical Looping Approach. *Energy Technology*, 4(10), 1200-1208.

# POWER GENERATION AND DISTRIBUTION

## Overview:

An effective, resilient electric power system is essential to the economic and energy security of the U.S. Many different factors are driving the need for modernization and diversification of the electric power system. These include the need to modernize the transmission and distribution of electric power, the desire for local autonomy in producing electric power, and the compelling need for safe, clean, and cost-effective power generation technologies that will reduce GHG emissions. ARPA-E has supported innovative approaches to modernize all aspects of the system, including distribution, cost-effective carbon dioxide capture from thermoelectric power plants burning fossil fuels, and novel approaches to capturing electric power regionally.

Thermoelectric power plants currently account for over 37% of all U.S. emissions of carbon dioxide. Post-combustion carbon capture, in which the CO<sub>2</sub> is separated from other flue gases (primarily nitrogen), is technically challenging and reduces the overall efficiency of power production. The “Innovative Materials and Processes for Advanced Carbon Capture Technologies, or IMPACCT program (2010) sought new technologies that could reduce the parasitic loads (steam and power) required to support CO<sub>2</sub> capture at scale while minimizing the impact on the levelized cost of electricity (LCOE).

ARPA-E’s OPEN solicitations have yielded innovative and exciting projects in the area of power distribution and generation. These projects have allowed the agency to explore innovative new technologies to develop new measurement technologies to monitor and more efficiently control power transmission and distribution on the grid and to more effectively convert solar, wind, and hydrokinetic energy into electricity.

The examples below represent the diversity and creativity of projects in power generation and distribution:

- RTI International (IMPACCT) – Carbon Capture with Water-Free Solvents
- Lawrence Berkeley National Laboratory/University of California, Berkeley (IMPACCT) – Novel Metal-Organic Framework Sorbents for Carbon Capture
- General Electric (OPEN 2012) – Back to the Future, for the Electric Power Grid
- University of California, Berkeley (OPEN 2012) – Precise, Time Synchronized Distribution Grid Measurements
- Brown University (OPEN 2012) – Self-Optimizing River and Tidal Power Conversion Devices
- Integral Consulting (OPEN 2012) – Low-Cost, Real-Time Wave-By-Wave Assessment Tool
- Otherlab (OPEN 2012) – Pneumatically-Actuated PV Tracking System Reduces Cost and Improves Reliability
- Glint Photonics (OPEN 2012) – Low-Power Microscale Tracking for Low-Profile Daylighting

# CARBON CAPTURE WITH WATER-FREE SOLVENTS

Updated: January 19, 2017

<b>PROJECT TITLE:</b> Novel Non-Aqueous CO <sub>2</sub> Solvents and Capture Process with Substantially Reduced Energy Penalties
<b>PROGRAM:</b> Innovative Materials and Processes for Carbon Capture Technologies (IMPACCT)
<b>AWARD:</b> \$2,480,000
<b>PROJECT TEAM:</b> RTI International (Lead), BASF
<b>PROJECT TERM:</b> July 2010 – September 2013
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Luke Coleman

## TECHNICAL CHALLENGE

U.S. thermoelectric power plants burning fossil fuels release over two billion tons of carbon dioxide (CO<sub>2</sub>) annually—37% of all U.S. emissions. Strategies for carbon capture and storage (CCS) figure prominently in most approaches to a deep-decarbonization energy future. Post-combustion carbon capture, in which the CO<sub>2</sub> is separated from other flue gases (primarily nitrogen), is the likely first approach because it is most readily retrofitted to existing plants. However, CCS represents a significant cost to power plants, as current technologies would increase the cost of electricity by approximately 80%. This increase is due to high capital costs as well as the energy required: 2.6 gigajoules to capture one ton of CO<sub>2</sub> with the standard commercial amine process.

## TECHNICAL OPPORTUNITY

The first step in CCS, CO<sub>2</sub> capture, is a significant technical challenge and the most expensive part of the process. CO<sub>2</sub> today is captured industrially by amine solvents. These solvents selectively bind CO<sub>2</sub>, but they are highly corrosive and must be heated to 120 degrees Celsius to release the captured CO<sub>2</sub> and regenerate the solvent. The heat is supplied by steam generated at a power plant that would otherwise be used to produce power. The corrosive nature of the amine solvent necessitates mixing it with a large amount of water that must be heated and cooled as part of the overall capture process. Capturing CO<sub>2</sub> without requiring such large volumes of water could increase the efficiency and greatly reduce the cost of CCS.

## INNOVATION DEMONSTRATION

The RTI team's goal was to develop a non-aqueous solvent (NAS) that does not need to be mixed with water, with the potential to reduce the energy cost of CO<sub>2</sub> capture by 20-30% compared with the current amine process. To do so, the team screened a large number of solvents to identify candidates with (a) low water solubility to avoid excess water uptake, (b) low vapor pressure to reduce solvent losses, (c) low heat capacity to minimize the energy required to regenerate the solvent, and (d) low corrosivity. This screening process identified 15 such candidates. After further testing, RTI selected 5 solvents that could potentially meet the target of being regenerated at temperatures below 120 °C, the current minimum temperature required for amine solvents.

Finally, RTI conducted longer-term testing of the most promising solvent composition, designated NAS-2. NAS-2 was tested for over 600 hours in simulated flue gas, which included contaminants such as sulfur dioxide. The team concluded that with some sulfur cleanup at power plants, the degradation rate of their solvent would be no more than 1% per 100 hours. RTI conducted a techno-economic analysis to estimate the expected performance of the NAS-2 solvent in a representative power plant, relative to the amines used today; they concluded that NAS-2 could be 20-30% better in terms of the parasitic energy penalty than current technology. In



Figure 1: RTI's bench-scale solvent testing unit.

parallel, RTI built a larger-scale test facility at its campus in North Carolina, featuring a 35-foot high absorber column capable of capturing 185 kilograms of CO<sub>2</sub> per day, more than 100 times the capacity of RTI's smaller lab-scale system. Evaluations of the candidate solvents in this facility continued after ARPA-E funding ended, as described below.

## PATHWAY TO ECONOMIC IMPACT

Following completion of the ARPA-E project, RTI initiated a follow-on collaboration with Linde, LLC and was awarded federal funding by the National Energy Technology Laboratory (NETL) in 2013 to refine the NAS solvents and test them in the larger facility equipment. The RTI team first tested a conventional amine solvent in the large facility to establish baseline data, then tested RTI's most recent NAS formulation on simulated flue gas and in an optimized process configuration. Several hundred hours of bench scale testing have been completed. The results indicate that the NAS technology can reduce the energy required to less than 2 gigajoules per ton of CO<sub>2</sub>, which is consistent with RTI's early projections of a 20-30% reduction in energy required compared to state of the art. Solvent degradation was found to be within acceptable limits.

Following that project, RTI received additional federal funding from NETL to scale the RTI NAS process up to a 60 kW facility in collaboration with SINTEF, a Norwegian research company. RTI will test a baseline formulation at the SINTEF test site in Norway, before applying the RTI optimized NAS. The SINTEF facility is being outfitted with a multiburner that allows, for the first time, testing of NAS in coal-derived flue gas. The results will be used to create a more accurate projection of the CO<sub>2</sub> capture cost for this promising new solvent.

## LONG-TERM IMPACTS

The RTI project with ARPA-E and the continuing work at NETL have demonstrated significant potential to lower the cost of carbon capture in coal-fired power plants compared with the incumbent amine technology. RTI's non-aqueous solvent could potentially reduce the energy required for carbon capture by 20-30%.

The technical feasibility and economic costs of carbon capture are an important input to policy decisions regarding greenhouse gas emissions. Since 2009, the technical understanding of the performance potential and associated costs for carbon capture have expanded significantly, but policy-makers' analyses of carbon capture costs are still shaped by the amine-based process. The work of DOE's Office of Science, Office of Fossil Energy and ARPA-E is expanding the pipeline of innovative new approaches to capture CO<sub>2</sub>. The next few years of continuing development will establish where there are realistic options to lower the costs of industrial carbon capture sufficiently to make new processes economically attractive. As such work progresses, the outcome of investments in innovation in this field will begin to inform future policy decisions concerning carbon capture and its role in addressing climate change.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of September 2016, the ARPA-E funding to the RTI/BASF team has resulted in four disclosures, four U.S. Patent and Trademark Office (PTO) patent applications, and one issued patent:

### Patent:

Katz, T. "REMOVING SULPHUR OXIDES FROM A FLUID STREAM" (2014). US Patent No. 8,691,171. Washington, DC: U.S. Patent and Trademark Office.

The RTI team has also published the scientific underpinnings of this technology in the open literature, listed below, and presented at numerous conferences.

### Publication:

"Non-Aqueous Solvent (NAS) CO<sub>2</sub> Capture Process," M. Lail, J. Tanthana, L. Coleman, 12th International Conference on Greenhouse Gas Control Technologies, (GHGT-12), 63, 580-594, 2014

# NOVEL METAL-ORGANIC FRAMEWORK SORBENTS FOR CARBON CAPTURE

Updated: October 5, 2016

<b>PROJECT TITLE:</b>	High-Throughput Discovery of Robust Metal-Organic Frameworks for CO <sub>2</sub> Capture	Developing Metal-Organic Frameworks as Adsorbents for Industrial Carbon Capture Applications
<b>PROGRAM:</b>	Innovative Materials and Processes for Advanced Carbon Capture Technologies (IMPACCT)	
<b>AWARD:</b>	\$3,867,851 (LBNL)	\$1,100,000 (UC Berkeley)
<b>PROJECT TEAM:</b>	University of California, Berkeley (Lead); Lawrence Berkeley National Laboratory (Lead); Wildcat Discovery Technologies, ADA-Environmental Solutions; Electric Power Research Institute	
<b>PROJECT TERM:</b>	August 2010 – August 2013 (LBNL)	September 2013 – September 2015 (UC Berkeley)
<b>PRINCIPAL INVESTIGATOR (PI):</b>	Dr. Jeffrey Long	

## TECHNICAL CHALLENGE

In carbon capture and storage (CCS), selective separation of CO<sub>2</sub> from exhaust gas is technically challenging, and all capture processes require energy, which reduces the overall efficiency of power production. Challenges in bringing new technologies to implementation are: (1) demonstration at the scale necessary for power plant application; (2) reduction of the parasitic loads (steam and power) required to support CO<sub>2</sub> capture that significantly decrease power generating capacity; and (3) reduction of the costs of scaled-up processes to minimize impact on the levelized cost of electricity (LCOE).

## TECHNICAL OPPORTUNITY

The commercially demonstrated technology for capture uses chemical absorption of CO<sub>2</sub> with a monoethanolamine (MEA) solvent. The parasitic energy cost is estimated to be 22-30% of the power plant output, and the projected increase in LCOE is ~80% for a supercritical pulverized coal plant. The Department of Energy (DOE) goals for carbon capture call for removing 90% of the CO<sub>2</sub> from power plant exhaust with no more than a 35% increase in the LCOE. Alternative approaches to selective, low-cost carbon capture include solid sorbents, which temporarily bind CO<sub>2</sub> through physical or chemical interactions for subsequent release. Metal-organic frameworks (MOFs), crystalline compounds composed of metal ions linked by organic molecules in a highly porous, three-dimensional network (see Figure 1),<sup>9</sup> are a promising class of sorbents. Because of the rich diversity in the various combinations of metal ions and organic linkers, MOFs offer opportunities to tune their properties to selectively bind CO<sub>2</sub> with minimum energy cost and to withstand the harsh post-combustion environment. Developing and testing of these materials can be greatly accelerated using new high-throughput screening approaches.

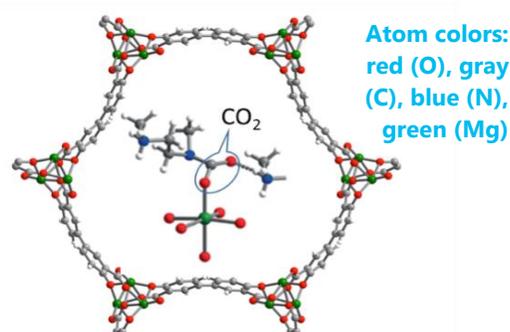


Figure 1: MOF pore structure (diamine groups not shown); inset shows CO<sub>2</sub> adsorption through insertion into a metal-amine bond.

<sup>9</sup> McDonald, T. M. et al. "Cooperative insertion of CO<sub>2</sub> in diamine-appended metal-organic frameworks" Nature 519, 303-308, doi: 10.1038/nature14327 (2015).

## INNOVATION DEMONSTRATION

Under ARPA-E support, Lawrence Berkeley National Laboratory (LBNL), in conjunction with the University of California at Berkeley (UCB), Wildcat Discovery Technologies, and the Electric Power Research Institute (EPRI), set out to synthesize and characterize MOF sorbents for carbon capture applications. The approach was for Wildcat to construct and validate a custom-designed, high-throughput system capable of measuring mixed gas isotherms for 28 samples in parallel and for the UCB team to use it to synthesize and characterize new MOFs which selectively adsorb large quantities of CO<sub>2</sub> at low partial pressures. The system is designed to provide isotherm measurements, which allow for identification of promising sorbents. The high-throughput system was designed to mix a number of gases and control the humidity while maintaining a high level of precision, thus allowing the UCB team to rapidly screen materials for a variety of flue gas conditions.

As the project progressed, UCB was joined by ADA-Environmental Solutions (ADA-ES) and the team worked to fine tune a particular class of MOFs and identify their capability as sorbents in power plant applications. Throughout both projects, the team was able to leverage the materials discovery research supported by the DOE Office of Science, Office of Basic Energy Sciences (BES) within the *Center for Gas Separations (CGS)*, an Energy Frontier Research Center. The CGS was responsible for the initial discovery of a promising class of MOF sorbents that have 18-nm-wide channels (Figure 1) with accessible metal surface sites that can be decorated with diamines and subsequently act as binding sites to insert CO<sub>2</sub> molecules (Figure 1 inset). The unique characteristic of these stable MOFs is reflected by the sharp step in the CO<sub>2</sub> adsorption isotherms, which measure CO<sub>2</sub> uptake as a function of pressure at fixed temperature (Figure 2b). Compared to a typical sorbent (Figure 2a), the amine-appended MOF-based sorbent (Figure 2b) exhibits a much higher working capacity (the amount of CO<sub>2</sub> removed) for a given temperature swing. This unusual isotherm results from reorganization of the appended amines into well-ordered chains of ammonium carbamate, resulting from chemical insertion of CO<sub>2</sub> molecules (Figure 1 inset).

The unique MOF isotherm represents an opportunity to reduce the parasitic energy load of CCS. Because the pressure at which the material demonstrates this step change depends upon the exact structure of the MOF, they are excellent candidates for rapid screening of numerous MOF compositions. The UCB team varied the MOF metal center (Mg, Mn, Fe, Co, and Zn) and the structure of the amine to identify the materials that perform best under realistic carbon capture conditions. The high-throughput system developed under the ARPA-E award allowed rapid collection of data at a large number of temperatures and partial pressures of CO<sub>2</sub> for over 100 MOFs. The resulting data was combined with a carbon capture model for coal-fired plants, developed by EPRI, to further assess and screen MOFs based on adsorbent energy in an optimized power-plant process. The models and materials were then further optimized with additional input from ADA-ES on realistic plant operating conditions.

Through this collaboration, UCB developed an MOF capable of selectively adsorbing CO<sub>2</sub> from a typical coal plant exhaust stream and desorbing at only moderately higher temperature. The significance of this result is apparent in the EPRI models, which predict a decrease in parasitic energy penalty from 30% for traditional processes to 15% for an optimized MOF with a different appended amine. The UCB team also demonstrated scalability of the optimized adsorbent to over 300 g and prepared a pelletized form that is suitable for testing in fixed bed reactors. Testing in this environment will generate long-term cycle and thermal stability data in addition to more realistic sorption properties. ARPA-E support has enabled development of these novel systems from a BES materials discovery, through optimization for CO<sub>2</sub> capture, and a path toward production and optimization on a commercial scale.

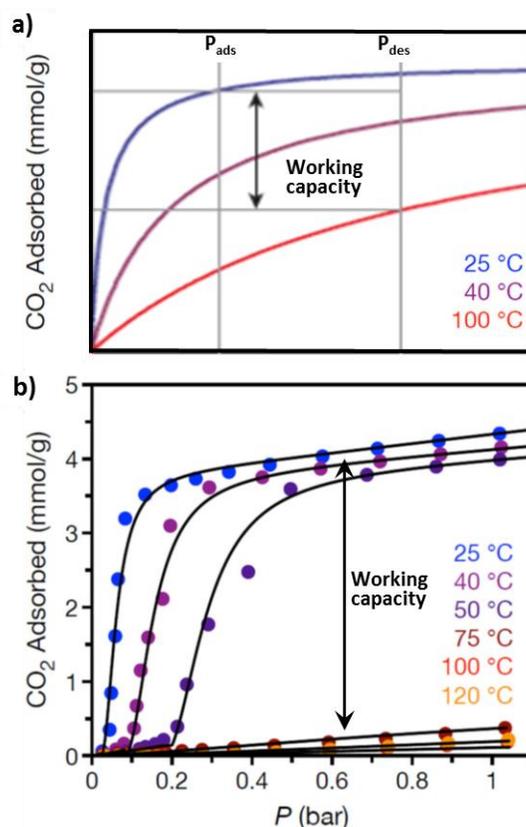


Figure 2: a) Idealized CO<sub>2</sub> adsorption isotherms at three temperatures; b) isotherms of a MOF with step-like adsorption. The double-headed arrows indicate the working capacity.

## PATHWAY TO ECONOMIC IMPACT

A new company, Mosaic Materials, was spun out of UCB in June of 2014 to develop an inexpensive means of producing the new CO<sub>2</sub> capture materials on the ton scale in a pelletized form. The initial funding was provided through Cyclotron Road at LBNL, which provides promising innovators with the tools, capital, and partners needed to commercialize their technologies. Mosaic Materials has since received funding from the California Energy Commission to develop a low-cost material capable of upgrading biogas streams to pipeline quality by scrubbing CO<sub>2</sub> and from the Office of Naval Research to scrub CO<sub>2</sub> from the atmosphere of submarines. Mosaic Materials also recently closed a \$1.5M Series A funding round with Evok Innovations, which will enable them to further scale up and gain traction in the marketplace. Finally, the Long group at UCB has received funding from two oil and gas firms and a start-up company to investigate the fundamentals of new materials relevant to related CO<sub>2</sub> separations, both by using the specific MOF system developed under this project and by applying the high-throughput discovery technology to fine tune other new materials for specific applications.

## LONG-TERM IMPACTS

The novel class of adsorbents based on diamine-appended MOFs produced by UCB holds promise for cost-effective carbon capture in the future, as well as energy-efficient applications in related industrial processes. In addition, the high-throughput analysis platform developed by Wildcat Discovery Technologies has the potential to rapidly screen numerous promising compounds under different conditions, mimicking conditions of flue gas from power plants and directly impacting the commercial viability of new adsorbents. Further improvements in related innovative adsorbent technologies for industrial carbon capture are possible. Implementation of such CCS technologies are enabled by the types of cost and performance improvements demonstrated for MOFs, but will also depend on policy decisions to move beyond demonstration and first-markets to widespread applications in thermoelectric power generation.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of July, 2016, the team's project has generated two invention disclosures to ARPA-E, two U.S. Patent and Trademark Office (PTO) patent applications, and two U.S. PTO issued patents.

### Patents:

"Cooperative Chemical Adsorption of Acid Gases in Functionalized Metal-Organic Frameworks" (2015) U.S. Patent No. WO2015164543 A1. Washington, DC: U.S. Patent and Trademark Office

"Apparatus for Gas Sorption Measurement with Integrated Gas Composition Measurement Device and Gas Mixing" (2014) U.S. Patent No. 8,739,603 B2. Washington, DC: U.S. Patent and Trademark Office

The team has also published the scientific underpinnings of this technology extensively in the open literature. A list of patents and publications is provided below:

### Publications:

Mason, J. A., McDonald, T. M., Bae, T.-H., Bachman, J. E., Sumida, K., Dutton, J. J., Kaye, S. S., & Long, J. R. "Application of a High-Throughput Analyzer in Evaluating Solid Adsorbents for Post-Combustion Carbon Capture via Multicomponent Adsorption of CO<sub>2</sub>, N<sub>2</sub>, and H<sub>2</sub>O" *Journal of the American Chemical Society* 137, 4787-4803, doi:10.1021/jacs.5b00838 (2015).

McDonald, T. M. et al. "Cooperative insertion of CO<sub>2</sub> in diamine-appended metal-organic frameworks" *Nature* 519, 303-308, doi: 10.1038/nature14327 (2015).

McDonald, T. M., Bloch, E. D. & Long, J. R. "Rapidly assessing the activation conditions and porosity of metal-organic frameworks using thermogravimetric analysis" *Chemical Communications* 51, 4985-4988, doi: 10.1039/C5CC00681C (2015).

Chen, J. J., Mason, J. A., Bloch, E. D., Gygi, D., Long, J. R., & Reimer, J. A. "NMR relaxation and exchange in metal-organic frameworks for surface area screening" *Microporous and Mesoporous Materials* 205, 65-69, doi: 10.1016/j.micromeso.2014.07.037 (2015).

Kim, J., Abouelnasr, M., Lin, L.-C., Smit, B. "Large-Scale Screening of Zeolite Structures for CO<sub>2</sub> Membrane Separations" *Journal of the American Chemical Society* 135, 7545-7552, doi: 10.1021/ja400267g (2013).

Swisher, J. A., Lin, L.-C., Kim, J. & Smit, B. "Evaluating mixture adsorption models using molecular simulation" *AIChE Journal* 59, 3054-3064, doi:10.1002/aic.14058 (2013).

Sathre, R. & Masanet, E. "Prospective life-cycle modeling of a carbon capture and storage system using metal-organic frameworks for CO<sub>2</sub> capture" *RSC Advances* 3, 4964-4975, doi: 10.1039/C3RA40265G (2013).

Chen, J. J. et al. "Ex Situ NMR Relaxometry of Metal-Organic Frameworks for Rapid Surface-Area Screening" *Angewandte Chemie* 52, 12043-12046, doi:10.1002/anie.201305247 (2013).

Bae, T.-H. et al. "Evaluation of cation-exchanged zeolite adsorbents for post-combustion carbon dioxide capture" *Energy & Environmental Science* 6, 128-138, doi: 10.1039/C2EE23337A (2013).

Sathre, R., Chester, M., Cain, J. & Masanet, E. "A framework for environmental assessment of CO<sub>2</sub> capture and storage systems" *Energy* 37, 540-548, doi: <http://dx.doi.org/10.1016/j.energy.2011.10.050> (2012).

Lin, L.-C. et al. "In silico screening of carbon-capture materials" *Nature Materials* 11, 633-641, doi: 10.1038/nmat3336 (2012).

Kim, J. et al. "Large-Scale Computational Screening of Zeolites for Ethane/Ethene Separation" *Langmuir* 28, 11914-11919, doi:10.1021/la302230z (2012).

Abouelnasr, M. K. F. & Smit, B. "Diffusion in confinement: kinetic simulations of self- and collective diffusion behavior of adsorbed gases" *Physical Chemistry Chemical Physics* 14, 11600-11609, doi: 10.1039/C2CP41147D (2012).

Mason, J. A., Sumida, K., Herm, Z. R., Krishna, R. & Long, J. R. "Evaluating metal-organic frameworks for post-combustion carbon dioxide capture via temperature swing adsorption" *Energy & Environmental Science* 4, 3030-3040 doi:10.1039/C1EE01720A (2011).

# BACK TO THE FUTURE, FOR THE ELECTRIC POWER GRID

Updated: February 3, 2017

<b>PROJECT TITLE:</b> High-Voltage, High-Power Gas Tube Technology for HVDC Transmission
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$7,206,569
<b>PROJECT TEAM:</b> General Electric Company (Lead), University of Wisconsin, Princeton Plasma Physics Lab
<b>PROJECT TERM:</b> April 2013 – April 2017
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Timothy J Sommerer

## TECHNICAL CHALLENGE

Direct-current (DC) electric power transmission is an enabling technology for improved security of the electric power system through long-distance power transmission, connecting asynchronous grids, and integration of renewable energy onto the grid. The cost-per-mile of a traditional high-voltage alternating current (HVAC) overhead line is 25–100 percent higher than a corresponding High Voltage DC (HVDC) line. However, DC power transmission requires that generated AC power be rectified to DC for transmission, and then inverted back to AC for customers. Existing AC-DC power conversion equipment is mature but expensive, limiting the beneficial use of DC systems. A more cost-effective conversion technology is needed.

## TECHNICAL OPPORTUNITY

Physical gas tube devices—gas-tight assemblies of metal electrodes and ceramic insulators—were the original means for high-voltage grid-scale AC-DC power conversion. They were displaced by power semiconductors, because of their superior reliability and lower maintenance requirements. A disadvantage of power semiconductors is that their voltage-handling capability is modest (<10 kV) in view of the system voltage requirements (>300 kV). The high cost of present AC-DC converter equipment is caused in part by the complexity of stacking semiconductor power electronic devices in series to control very high system voltages. The trend is to even greater system complexity, as system voltages rise faster than device voltages, and systems are extended to applications with weak or nonexistent AC grids (e.g., offshore). However, tube devices have continued to be the technology of choice for demanding applications like x-ray tubes for medical imaging and microwave power tubes for satellite communications. Decades of technology development in those fields have led to vast improvements in tube reliability and performance. Thus, there is the opportunity to “go back to the future” and develop a modern gas tube for grid-scale power conversion.

## INNOVATION DEMONSTRATION

The goal of this project is to develop a long-life, high-voltage switching gas-plasma tube, capable to >300 kV. To achieve this goal the team has accomplished three major tasks, namely, the development of non-mercury liquid cathode and plasma, the scaling of device voltage, and the use of a low-loss mode of operation.

The first key component to the project approach is a self-healing liquid metal cathode. Even with all the advances in tube technology, physical damage to the cathode (negative electrode) is still expected to unacceptably limit device life for grid applications. The project’s approach is to replace the conventional solid metal cathode with a liquid metal cathode, with the idea that liquid metal can reflow and self-heal from some damage, and it can be pumped and replenished if necessary. The project team demonstrated that a liquid metal cathode could operate at the high current density (5 A/cm<sup>2</sup>) required for grid applications, based on the technological developments that now underpin the use of liquid metal bearings in some high-voltage x-ray tubes.

A second focus of the project is the scaling of device voltage. A crossed field (electric and magnetic field) device design was selected as the starting point, and the team has built and operated such devices to 100 kV. Device testing within the

project is limited by power considerations to single-pulse operation. The team is now constructing and expecting to demonstrate operation of a 300 kV device and to estimate the upper limit of the operating voltage for this technology.

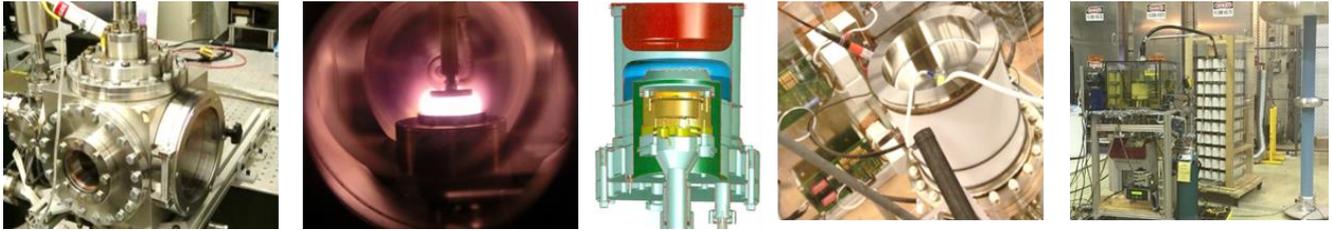


Figure 1: Montage of experimental work performed within the current Project. (a) 'Benchtop' system for liquid cathode development; (b) interior of Benchtop system during conduction phase operation; (c) Gas Switch device cut-away; (d) Gas Switch with Power Electronic Controls in background; (e) 300 kV test facility used for 100 kV Switch testing (Switch is immersed in yellow transformer oil, capacitor bank is in the background).

During the project, the team found that the tube can operate in a unique low-loss low-voltage mode that could have great benefits for both life and efficiency. The device efficiency improves as the device dissipates less power during on state with the lowered forward voltage. The device reliability improves since the wear-out mechanism of the cathode is exponentially dependent on the forward voltage.

The team evaluated several system topologies to estimate the cost, efficiency, and size of a system for long-distance DC transmission by overhead wires. For the base case (3 GW, 500 miles) the team found that the AC-DC conversion equipment cost could be halved if the tube operating voltage could be increased to 300 kV. An important part of the cost savings arises because the system topology produces a cleaner AC waveform, and less filtering is needed.<sup>10</sup> The efficiency of the system is expected to be competitive with, or even slightly better than, the best thyristor-based systems.

## PATHWAY TO ECONOMIC IMPACT

General Electric develops and sells HVDC systems through its Grid Solutions business, which is initiating work in 2017 to build appropriate controls for a tube operation in a test-system environment, toward the goal of full-speed "burst" operation and testing. If successful, further tube testing will be done on a circulating-power facility capable of sustained full-speed operation, prior to the construction of a larger-scale demonstrator system. There is still at least 5 years of work to be done to move the technology from the laboratory onto the grid.

In the shorter term, gas tubes might be a good candidate for high-voltage protection devices on AC transmission lines. Niche markets such as this are useful for gaining field experience with the gas tube. In the longer term, the small size and lightweight of gas-switch tubes may have large benefits for specialized applications such as offshore AC-DC converters, which can be the size of oil platforms, and for city-center cable in-feeds, where real estate is at a premium. Gas-switch tubes can be part of a hybrid DC circuit breaker, a device that is complex and costly at this time, but is required for the emergence of a true DC grid.

## LONG-TERM IMPACTS

The gas tube technology developed and demonstrated in this project is expected to reduce overall HVDC terminal cost by 40%, potentially reducing the economically advantageous HVDC transmission distance relative to traditional AC infrastructure from 500 miles to 250 miles. GE's gas switches could also enable multi-terminal HVDC networks. Making HVDC transmission more economic could bolster new possibilities such as interties between regional grids for wider area balancing, and high-efficiency transmission corridors to reach remote areas with abundant solar or wind resources.

As there are currently no major power semiconductor manufacturers in North America due to high entry barriers and commoditized products, successful development of GE's gas switch technology promises to create high quality jobs in

<sup>10</sup> Physics Today (Magazine): Kim Krieger, 'A New Twist on an Old Technology', 13 Aug 2014

the U.S. for system innovation, manufacturing, and deployment of high-efficiency HVDC transmission components and infrastructure.

## **INTELLECTUAL PROPERTY AND PUBLICATIONS**

As of January 2017, the project has reported eight invention disclosures to ARPA-E, leading to seven patent applications and three issued patents.

### **Patents:**

Method and system for a gas tube switch-based voltage source high voltage direct current transmission system, US Patent 9,520,801

Systems and methods for regulating pressure of a filled-in gas, US Patent 9,330,876

Helium supply reservoir with fine dosing capability for an HVDC plasma switch, US Patent 9,557,009

The Project Team has also made numerous presentations of the scientific underpinnings of this technology at various scientific conferences, and has begun to publish findings in the open literature. The first publication is provided below:

### **Publication:**

Carlsson, J., Khrabrov, A., Kaganovich, I., Sommerer, T., & Keating, D. (2016). Validation and benchmarking of two particle-in-cell codes for a glow discharge. *Plasma Sources Science and Technology*, 26(1), 014003.

# PRECISE, TIME SYNCHRONIZED DISTRIBUTION GRID MEASUREMENTS

Updated: September 9, 2016

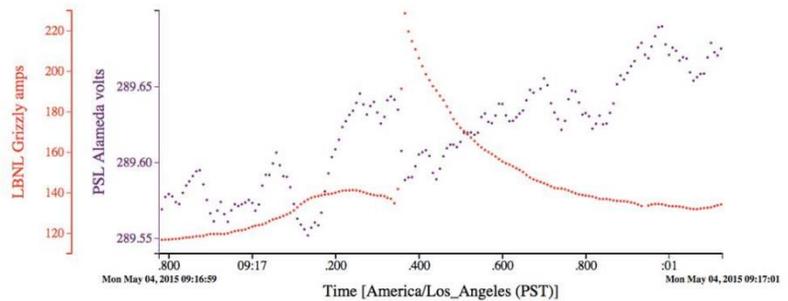
<b>PROJECT TITLE:</b> Micro-Synchphasors for Distribution Systems
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$3,892,276
<b>PROJECT TEAM:</b> University of California Berkeley/California Institute for Energy and Environment (Lead); Lawrence Berkeley National Lab; Power Standards Lab
<b>PROJECT TERM:</b> April 2013 – August 2016
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Alexandra von Meier

## TECHNICAL CHALLENGE

The distribution grid that delivers electric power to customers is changing rapidly. Historically, it has been relatively simple, predictable, and had little need for real-time diagnostic capabilities. But the advent of distributed energy resources (DERs) and new types of loads such as electric vehicles makes the operation of power distribution systems a growing challenge. Fully realizing the emissions, reliability and cost benefits of DERs will require real-time monitoring of distribution system behavior, using synchrophasor measurements similar to those available in higher voltage transmission networks. Yet monitoring the distribution system is more difficult because the required measurements are far more precise and also more numerous than in the transmission system. Addressing these challenges requires technical advances enabling useful, ultra-precise measurements on the distribution grid and methods to assess and act on the resulting complex data sets.

## TECHNICAL OPPORTUNITY

The ability to combine high-quality electrical measurements with the time accuracy of GPS and wireless communications into a network of micro-phasor measurement units ( $\mu$ PMUs) or micro-synchphasors provides new opportunities to monitor and control electricity distribution systems. Furthermore, advances in “big data” management tools and grid optimization algorithms make it possible to leverage the measurements from new sensor systems in important ways. The opportunities for applications include (1) supporting distribution system planning and operation functions related to utility owned infrastructural hardware, (2) supporting diagnostics of transmission system conditions from a larger number of measurement nodes, and (3) supporting the control of distributed energy resources—including generation, load, and storage—to realize their vast potential benefits for the grid.



**Figure 1:** Sample  $\mu$ PMU data illustrating the impact of a small current surge at two different locations approximately 40km apart. *Precise time synchronization and ultrahigh resolution is required to observe these kinds of relationships in distribution systems.*

## INNOVATION DEMONSTRATION

The primary objectives for this project included both the development and testing of  $\mu$ PMU hardware and the exploration and validation of potential  $\mu$ PMU data applications that would be valuable for utilities. To achieve the resolutions and sensitivities required for distribution system measurement, the project developed a new, unified and commercially deployable sensor. The project team also had to build a completely new database infrastructure for high-resolution time synchronized data to enable processing and analysis of  $\mu$ PMU data streams. Existing tools for the analysis of time-series data were either too slow or had limited scalability for handling this type of data.

To address the hardware challenges, the team developed new firmware for the existing “PQube” power quality measurement device and integrated it with a GPS receiver in order to achieve extremely high precision and temporal resolution. The team verified the performance and accuracy of the  $\mu$ PMU, demonstrating phase angle measurements with a resolution better than 10 millidegrees, an improvement of two orders of magnitude over standard transmission synchrophasors, at substantially reduced cost. The team tested and deployed an integrated network of 44  $\mu$ PMUs both within the lab and in various field settings with five partner utilities and gathered tens of terabytes of data from the devices.

For the database development project thrust, the team developed an innovative software technology named Berkeley Tree Database (BTrDB). BTrDB collects and stores many concurrent high-bandwidth, potentially unordered data streams 1400 times faster than the best previously available commercial solution. The database, which achieves a 2.9-time compression ratio, has demonstrated a throughput of 53 million inserts per second (ips) and 119 million queries per second on a four-node cluster. The novel data structure allows for extremely fast multi-scale analysis of data, thereby enabling prediction and anomaly detection across the range of voltage, current, and time-scales that affect distribution performance. For example, locating a handful of voltage sags in 3.4B data points comprising a year of data requires less than 200ms.



**Figure 2: A  $\mu$ PMU installed on a utility electric distribution pole. The device consists of a high-resolution power quality monitor and a GPS antenna (mounted on top of the box in this installation).**

Using  $\mu$ PMU data, the project team empirically characterized the steady-state and dynamic behavior of a set of electricity distribution circuits, developed a set of basic diagnostic applications, and laid the theoretical foundation for leveraging  $\mu$ PMU data in future control applications. The team’s study of early  $\mu$ PMU measurements revealed numerous conditions that were either unknown or suspected but not previously verifiable for distribution system operators. Through comparisons of empirical  $\mu$ PMU measurements with circuit models, the project team also identified key weaknesses of existing circuit models and tools as well as challenges for measurement accuracy under real-world field conditions. The team developed and validated several algorithms based on hypothetical  $\mu$ PMU input data including applications to calculate distribution state estimation, topology configuration, and fault location. The project team also developed early versions of working diagnostic tools with empirical  $\mu$ PMU data, including applications for model validation and for detection and classification of disturbance events (e.g. to identify causes of outages). These applications provided early value to the team’s utility partners. Conditions discovered or verified through  $\mu$ PMU measurements included high-impedance faults (e.g. arc flash or animal caused), reverse power flow, device malfunction, causes of voltage sags or load interruptions, and power and voltage oscillations at the transmission level. The team also developed and validated a methodology to estimate the real time generation behind the meter on a one minute basis to 6% root-mean-square error (RMSE) – significantly greater accuracy than state of the art weather based methods for real time generation estimation behind the meter.

With the completion of this project, the hardware and data processing infrastructure technology is in place to enable the development of utility-grade real-time distribution network monitoring and control applications. The team has also developed several proof-of-concept  $\mu$ PMU applications in the lab. The next critical step is the further development and testing of these applications to prepare them for validation with utilities. Testing and validation of algorithms in actual utility operations will be crucial to the next stage of development.

## PATHWAY TO ECONOMIC IMPACT

PSL has already begun to make commercial hardware sales of the  $\mu$ PMU<sup>11</sup> in the U.S. and internationally. Customers to date include Tesla, SolarEdge, the National Institute of Standards & Technology (NIST), Sandia National Lab, and researchers in Japan, Belgium, France and Poland. PSL plans to start selling  $\mu$ PMU Quick Start kits in 2016 that will include a small number of  $\mu$ PMU devices and the software needed to immediately start collecting and analyzing  $\mu$ PMU data.

The team has also identified a number of initial  $\mu$ PMU-based applications that they believe could be transitioned to utilities relatively quickly. Three commercialization partners, Smarter Grid Solutions, Doosan GridTech, and Ping Things, are facilitating development of utility-ready applications using  $\mu$ PMU data and/or the BTrDB software, which is being developed for release as open source. Initial applications will focus on giving utilities the tools to monitor and manage distribution feeders with high penetrations of photovoltaic generation and/or energy storage. The team is also working to improve the ability to perform real-time analysis and event detection on large-scale  $\mu$ PMU data streams.

In order to drive long-term impact through uniform standards, the team has spearheaded and chairs a distribution PMU working group at North American SynchroPhasor Initiative (NASPI), the governing body for synchrophasors in the U.S.  $\mu$ PMUs are also central to multiple related follow-on projects funded by the U.S. Department of Energy and Department of Defense that focus on topics including microgrids and cyber-security.

## LONG-TERM IMPACTS

When fully proven, applications using micro-synchrophasor measurements have the potential to create a transition from today's opaque, data constrained operating environment to one that is more fully information-enabled. Improved distribution state awareness will facilitate the integration of high penetrations of distributed energy resources.

Furthermore, the principles and design of the BTrDB database are generally applicable to a large variety of timeseries types and represent a significant advance in the development of technology for the Internet of Things.

As of 2016, the project has directly resulted in five full-time equivalent manufacturing jobs in California, anticipated to rise to 25 in 2017 and with the potential to reach 100 over the next five years.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of 2016, the project has generated one invention disclosure to ARPA-E, four U.S. Patent and Trademark Office (PTO) patent applications, and one patent:

### Patent:

*"System and method for measuring a parameter of an alternating current power grid while minimizing the likelihood of lightning damage in a measuring system,"* (2016), Patent No US9383397 B1, A. McEachern.

The open-source code for BTrDB is downloadable<sup>12</sup> and a subset of  $\mu$ PMU data are publicly viewable; a reference data set from LBNL is also to be released. The team has published the scientific underpinnings of this technology extensively in the open literature. A list of selected publications is provided below.

### Publications:

Micro-synchrophasor data for diagnosis of transmission and distribution level events, AL Liao, EM Stewart, EC Kara 2016 IEEE/PES Transmission and Distribution Conference and Exposition (T&D), 1-5. <http://ieeexplore.ieee.org/document/7519975/>

"Phasor Measurements for Distribution System Applications," Emma M. Stewart and A. von Meier, in Wiley Smart Grid Handbook, 2016. <http://onlinelibrary.wiley.com/doi/10.1002/9781118755471.sgd087/abstract>

Stewart, E. M., Kiliccote, S., McParland, C., Roberts, C., Arghandeh, R., & von Meier, A. (2014). Using Micro-Synchrophasor Data for Advanced Distribution Grid Planning and Operations Analysis. Ernest Orlando Lawrence Berkeley National Laboratory. <http://eetd.lbl.gov/publications/using-micro-synchrophasor-data-for-ad>

---

<sup>11</sup> [http://www.powersensorsltd.com/Download/MicroPMU%20Data%20Sheet%20Rev1\\_3.pdf](http://www.powersensorsltd.com/Download/MicroPMU%20Data%20Sheet%20Rev1_3.pdf)

<sup>12</sup> The open source code can be accessed here: <https://github.com/SoftwareDefinedBuildings/btrdb/>. More information about the code can be found here: <http://btrdb.io/>

"Accuracy and Model Validation of Measured and Modeled Data for Distributed PV Interconnection and Control," Emma M. Stewart, Sila Kiliccote, Daniel Arnold, Alexandra von Meier, Reza Arghandeh, 2015 IEEE PES General Meeting, Denver, CO 7, 2015. <http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=7286484>.

"BTrDB: Optimizing Storage System Design for Timeseries Processing," Michael P. Andersen and David E. Culler, 14<sup>th</sup> USENIX Conference on File and Storage Technologies. <https://www.usenix.org/conference/fast16/technical-sessions/presentation/andersen>

"Distribution Network Topology Detection with Time Series Measurement Data Analysis," G. Cavraro, R. Arghandeh, A. von Meier, IEEE Innovative Smart Grid Technologies (ISGT) Conference, 2015. <http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=7131897>

"Topology Detection in Microgrids with Micro-Synchrophasors," R. Arghandeh, M. Gahr, A. von Meier, G. Andersson, IEEE Power and Energy Society General Meeting 2015, Denver, CO 7, 2015. <https://arxiv.org/pdf/1502.06938.pdf>.

"DISTIL: Design and Implementation of a Scalable Synchrophasor Data Processing System," Michael P Andersen, Sam Kumar, Connor Brooks, Alexandra von Meier and David E. Culler, IEEE Smart Grid Communications Conference 2015, Miami, FL. <http://ieeexplore.ieee.org/document/7436312/?arnumber=7436312&tag=1>.

"Every Moment Counts: High Resolution Measurement for Distribution Network with Variable Sources," A. von Meier, R. Arghandeh, Renewable Energy Integration (Elsevier), 429-438 (2014). <https://arxiv.org/pdf/1408.1736.pdf>, <http://store.elsevier.com/Renewable-Energy-Integration/Lawrence-Jones/isbn-9780124079106/>.

"Micro-Synchrophasors for Distribution Systems," A. von Meier, D. Culler, A. McEachern, R. Arghandeh, IEEE Innovative Smart Grid Technologies (ISGT) Conference, Washington DC, USA 2, 2014. <http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=6816509>.

E. Stewart, S. Kiliccote, R. Arghandeh, A. von Meier, "Addressing the Challenges for Integrating Micro-Synchrophasor Data with Operational System Applications", IEEE Power & Energy Society General Meeting, National Harbor, MD, July 2014. <http://ieeexplore.ieee.org/document/6938994/>

# SELF-OPTIMIZING RIVER AND TIDAL POWER CONVERSION DEVICES

Updated: January 27, 2017

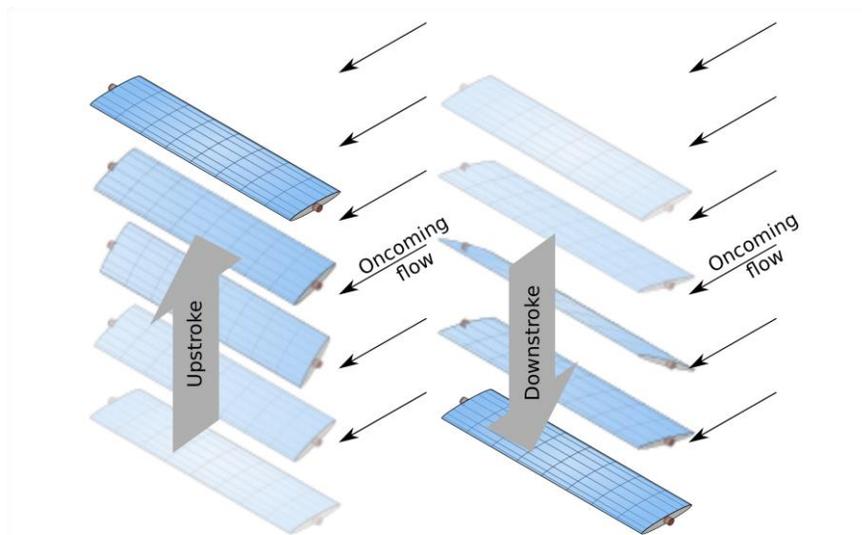
<b>PROJECT TITLE:</b> Marine Hydrokinetic Energy Harvesting Using Cyber-Physical Systems
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$3,659,924
<b>PROJECT TEAM:</b> Brown University (Lead), BluSource Energy, Volpe National Transportation Systems Center, Wellesley College
<b>PROJECT TERM:</b> March 2013 – May 2017
<b>PRINCIPAL INVESTIGATOR (PI):</b> Shreyas Mandre

## TECHNICAL CHALLENGE

Marine hydrokinetic energy conversion is a potential candidate for regionally sourced electricity, which can meet the security, economic, and environmental needs of local communities. Riverine and tidal energy converters show promise, but both are still nascent industries. These technologies are typically not cost competitive ( $> \$0.25/\text{kWh}$ )<sup>13</sup> because of the inherent drawbacks of passive, rotary turbine-based systems. Traditional rotary turbines suffer from three major challenges. First, they have limited scalability due to the fact that they must be sparsely distributed in a river or tidal field, as they are not compatible with shallow sites, and they do not efficiently extract power across all flow conditions. Second, traditional rotary turbines require specialized and expensive deployment and maintenance. Finally, they may lead to undesirable environmental effects. Traditional rotary turbines may interfere with animal movement and the turbine blades may pose risk of injury due to high tip speeds during rotation. New design approaches are required to overcome these drawbacks.

## TECHNICAL OPPORTUNITY

Studies in the field of fluid dynamics has shown that a number of flying insects, birds and animals outperform fixed wing aerodynamic performance using unsteady leading edge vortex shedding. This suggests that the unsteady effects themselves have the potential to improve the efficiency of power conversion by enhancing lift (delaying stall). If the leading edge vortex can be controlled this approach can be used to improve efficiency and cost-competitiveness of riverine and tidal energy conversion systems, which have traditionally aimed to avoid unsteady hydrodynamic flow regimes.



**Figure 1: Principle of operation behind power conversion by oscillating hydrofoil systems. The hydrofoil is tilted downwards on a down stroke (left) and upwards on an up stroke (right). As a result, the hydrodynamic force on the hydrofoil always points in the direction of the motion, and the flow does mechanical work on the hydrofoil, which drives a generator.**

<sup>13</sup> Neary, Vincent S., et al. "Methodology for design and economic analysis of Marine Energy Conversion (MEC) technologies." (2014).

## INNOVATION DEMONSTRATION

The Brown Team's goal was to incorporate active feedback and control into a physical tidal generator based on an oscillating hydrofoil design. The basic principle of operation of an oscillating hydrofoil, which is very different from a rotating turbine, is shown schematically in Figure 1. The primary objective was to demonstrate deployment, survivability and electricity generation at rated power over at least one month in reversing tidal flow.

The Brown team used lab experiments and computational fluid dynamics (CFD) analysis as a tool to design, optimize and validate the design. The result is a 1kW device with a mechanically coupled pair of wings that are driven by flowing water to heave vertically and pitch at the center axis. The optimal kinematics for the Leading Edge foils have a high pitching amplitude, or high maximum angle of attack (70-80 degrees). At these high angles, the boundary layer, or the fluid on the surface of the foil, separates from the surface and forms a vortex at the leading edge of the foil. This leading edge vortex persists over the top of the foil during the upstroke, increasing the lift force with its low pressure core for a large portion of the stroke. When the foil reserves at the top of the stroke the vortex sheds, and another is formed on the lower side of the foil for the same effect. A real-time controller monitors the position and forces on the wing and adjusts the load to maximize power output at a given flow speed.



**Figure 2: Brown University's 2kW prototype cyber-physical oscillating hydrofoil marine hydrokinetic energy generation system. (Left) Model of the floating platform design showing the generators, each with tandem hydrofoils, and their ability to pivot into and out of the water. (Right) Photograph of the fabricated device, before its multi-week deployment at the Massachusetts Maritime Academy.**

A second prototype test was conducted to test the interactions between two devices, the second downstream of the first. The pair of tandem foils illustrated in Figure 2 achieved the 2kW design power rating. The power generated by the downstream set of foils was 60-80% of that generated by the leading foils, as compared to rotary turbines where the trailing turbine generates at most 40% when placed 6 diameters away. Deployment used a low-cost tugboat that brought the floating platform into position and lowered the foils into the water. Seamless transition between operating mode (hydrofoils pivoted in) and maintenance mode (hydrofoils pivoted out) was demonstrated.

To assess potential environmental effects of the oscillating hydrofoil design, the Brown team formed a partnership with Wellesley College and the Volpe Center. Wellesley College, through a series of experiments, showed that under laboratory conditions the device had minimal impact on fish behavior or on biochemical indicators of physiological stress. The Volpe Center assessed the technology for a wide range of environmental considerations (alteration of currents and waves; alteration of bottom substrates, sediment transport, sediment deposition, and benthic habitats; noise; chemical toxicity; interference with animal movement or migration; and strike; amongst others). They identified several aspects of the hydrofoil design that may have reduced environmental impacts compared to traditional rotary turbines.

Field data from summer 2016 tests suggests that the effects of the technology on water currents is limited to a short distance below and behind the device, thus effects on sediment transport are likely minimal. Additionally, the tip speed of the foils was the same as the water speed while tip speed of rotary turbines is significantly faster than the water speed. Slower movement of hydrofoils for a given current speed compared to turbine blades is likely to be easier for wildlife to avoid, further reducing the risk for injury and mortality due to strike.

## PATHWAY TO ECONOMIC IMPACT

Market analysis revealed that the initial system should be designed to meet the need of smaller (kW) scale systems in remote off-grid markets (e.g. Alaska, Maine, and Brazil) that rely on shipped-in diesel fuel with >\$0.50/kWh energy costs. The technoeconomic analysis developed by the team estimates a levelized cost of electricity (LCOE) of approximately \$0.37/kWh at the 50kW scale, which would be disruptive to this first, and important, market. Once the team is able to achieve success in the remote off-grid market, it is likely that the next application for technology would be as a component of a microgrid, complementing diesel power and other non-baseload renewables like solar and wind. Combined, these two markets are conservatively estimated to be at least \$600M.

The project team has attracted a potential commercial partner in BluSource Energy. To secure additional funding, the next step would be to design, build and test a 10 kW prototype for one year, which is a standard milestone potential investors require. The Brown team is actively pursuing some recent federal funding opportunities directed toward such year-long tests.

## LONG-TERM IMPACTS

River and tidal energy conversion has the potential for approximately 600TWh/yr (about 16% of present U.S. power generation) in the United States<sup>14</sup>, almost all of which is currently untapped. This team's technical innovation has shown that next generation, cyber-physical riverine and tidal energy generation devices have the potential to viability for significantly lowered costs. Early deployment through first-markets such as remote off-grid communities, which have limited alternatives but abundant river and tidal resources, is viable, and would place the technology on a pathway to utility (MW) scale applications through economies of scale.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of October 2016, the Brown University team's project has generated two invention disclosures and a U.S. Patent and Trademark Office (PTO) patent application. The team has also published the scientific underpinnings of this technology in the open literature. One publication is provided below:

"Field-testing of a 1kW Oscillating Hydrofoil Energy Harvesting System," J. L. Cardona, M. J. Miller, T. Derecktor, S. Winckler, K. Volkmann, A. Medina, S. Cowles, R. Lorick, K. S. Breuer, and S. Mandre, Proceedings of the 4th Marine Energy Technology Symposium. 2016.

---

<sup>14</sup> <https://energy.gov/eere/water/marine-and-hydrokinetic-resource-assessment-and-characterization>

# LOW-COST, REAL-TIME WAVE-BY-WAVE ASSESSMENT TOOL

Updated: February 6, 2017

<b>PROJECT TITLE:</b> Cost Effective Real Time Wave Assessment Tool (WAT)
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$2,343,260
<b>PROJECT TEAM:</b> Integral Consulting (Lead), Sandia National Laboratory, Spoodrift Technologies
<b>PROJECT TERM:</b> September 2014 – August 2018
<b>PRINCIPAL INVESTIGATOR (PI):</b> Craig Jones and Grace Chang

## TECHNICAL CHALLENGE

Regionally sourced renewable electric power allows local communities to address their own needs while also supporting U.S. energy security and reducing energy emissions. One potential regional power source is wave energy, a form of marine hydrokinetic energy conversion<sup>15</sup> that shows promise. A wave energy converter (WEC) couples the motion of ocean waves into mechanical displacements that in turn drive an electric generator. The efficiency of energy capture relies on the WEC system being tuned to the frequency and amplitude of the waves, but ocean waves are highly variable. Early WEC systems used passive controls tuned to the average behavior of the waves and thus were able to capture only a fraction of the available power. As a result, the levelized cost of energy (LCOE) for WECs is not typically competitive.<sup>16,17,18</sup> New control approaches make it possible to actively tune a WEC system to the range of sea-states experienced (wave height and wave period combinations).<sup>19,20,21</sup> This requires highly accurate, real-time wave-by-wave measurements, which can be obtained by data buoys located in proximity to WECs. The cost of high-quality wave assessment buoys needs to be reduced by an order of magnitude to be cost effective for field deployment.

## TECHNICAL OPPORTUNITY

The WEC industry had prioritized active tuning research and funded the development of control algorithms and data protocols for wave measurements that can utilize buoy data. Recent advances from other technical fields have enabled innovative solutions to drive down costs in high-quality wave measurement systems. These include the availability of low-cost microprocessor control board technologies, as well as affordable GPS, accelerometer, gyroscope, and communication devices, and advanced real-time filtering techniques, capable of filtering large amounts of noisy electronic motion sensing data. In addition, very low cost and compact Computer Numeric Control manufacturing systems had become more widespread, enabling high precision, low-cost fabrication.

## INNOVATION DEMONSTRATION

The Integral team's project objective was to achieve wave-by-wave measurement accuracy comparable to commercial off the shelf (COTS) wave measurement devices for wave height, period, and direction at a tenth of the cost. The Integral team

<sup>15</sup> [http://en.openei.org/wiki/Marine\\_and\\_Hydrokinetic\\_Technology\\_Glossary](http://en.openei.org/wiki/Marine_and_Hydrokinetic_Technology_Glossary)

<sup>16</sup> OES (2015) International Levelised Cost of Energy for Ocean Energy Technologies, Ocean Energy Systems (OES)

<sup>17</sup> Previsic, Mirko, and Kourosh Shoele. "Cost-reduction pathways for wave energy." *Global Status and Critical Developments in Ocean Energy* (2012): 140.

<sup>18</sup> Neary, Vincent S., et al. "Methodology for design and economic analysis of Marine Energy Conversion (MEC) technologies." (2014).

<sup>19</sup> Belmont, M. R. (2010). Increases in the average power output of wave energy converters using quiescent period predictive control. *Renewable Energy*, 35(12), 2812-2820.

<sup>20</sup> F. Kara, "Time Domain prediction of power absorption from ocean waves with latching control.pdf." Elsevier Ltd., 2009

<sup>21</sup> Hals, J., Falnes, J., & Moan, T. (2011). A comparison of selected strategies for adaptive control of wave energy converters. *Journal of Offshore Mechanics and Arctic Engineering*, 133(3), 031101.

addressed this objective in two steps. The team first focused on cost reduction in their first generation product, and then outfitted the first generation device with wave-by-wave measurement capability.

The first technical challenge was the order-of-magnitude cost reduction of industry standard spectrally-based wave measurement buoys. The Integral team leveraged low cost microprocessor control board technologies and incorporated and synchronized accurate GPS, inertial measurement unit, and wireless data communication microelectromechanical systems technologies. The result was a spectral binning-based wave measurement buoy product, WaveSpotter V1, available at one-tenth the cost of state-of-art wave measurement systems.

The Integral team then embarked on the development of the next generation system to produce wave-by-wave measurements. One of the main challenges of wave-by-wave measurement is filtering the noisy data. To overcome this challenge, Integral leveraged advanced real-time filtering techniques developed primarily for the aerospace industry. The team validated the resulting wave measurement buoy, WaveSpotter V2, on a custom-built validation stand and demonstrated <5% error in derived displacement at 5 Hz and <1% error in period. The WaveSpotter V2 was also field-tested off the coasts of Waimanalo, HI and Santa Cruz and Santa Barbara, CA, where it demonstrated real-time communication of highly accurate (<5% difference compared to COTS devices), real-time, predicted wave data to another WaveSpotter that acted as a proxy WEC device.

In parallel, the team also developed a techno-economic model to quantify the impact on LCOE of a combined wave-by-wave assessment tool (WAT) + WEC array system vs a WEC array that did not incorporate a WAT. The analysis showed that the deployment of a low-cost, wave-by-wave WAT could provide significant gains in average annual power capture (up to 2 times) from a combination of increased power capture efficiency across all sea states and decreased duration of shut down periods. This could lead to a potential decrease of LCOE by as much as 50% compared to a WEC array that does not incorporate predictive control.

## PATHWAY TO ECONOMIC IMPACT

Integral plans to begin selling its first generation product, WaveSpotter V1, in early 2017. It is capable of generating wave data with resolution on the order of minutes and will be available at a low cost (~\$5,000). The Integral team is aiming at first-market applications including offshore oil and gas rig monitoring, maritime traffic, resorts and recreation, oceanic research and modelling, insurance industry, coastal protection, homeland security, and military applications. Success in these early markets will enable the team to scale production of the product.

Integral is working closely with WEC manufacturers to develop active tuning methodologies and protocols so that by the time WaveSpotter V2 is commercially ready, the market for it will be more fully developed. Additional field testing is planned for spring of 2017 to summer of 2017, where Integral will participate in joint demonstrations in which WEC devices will use predicted wave data from Integral's technology to actively tune themselves and test performance gains. If successful, Integral would be in position to quickly roll WaveSpotter V2 out to the market. WaveSpotter V2 can be produced in much the same way as WaveSpotter V1, allowing Integral to leverage the scaled-up WaveSpotter V1 production capability with simple substitution of the microprocessor unit and data telemetry system.

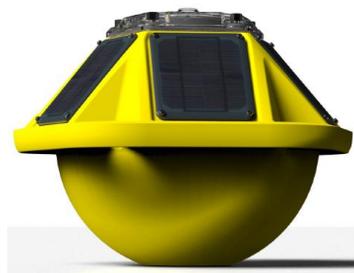


Figure 1: Integral's WaveSpotter V1. Unit height is 13 inches.

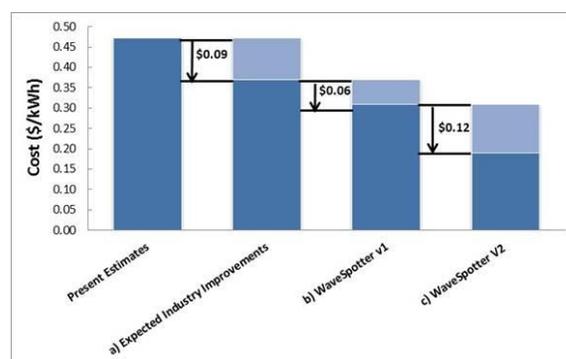


Figure 2: Estimated reductions in the LCOE of wave energy converters. Present estimates<sup>16,17,18</sup>, (a) expected industry improvements (not related to WaveSpotter)<sup>17</sup> (b) estimated benefit of incorporation of WaveSpotter v1 into the WEC array, (c) estimated benefit of incorporation of WaveSpotter v2 into the WEC array.

## LONG-TERM IMPACTS

Wave energy conversion has the potential to produce approximately 1,000TWh/yr (about 25% of the current domestic electricity generation)<sup>22</sup> in the United States, almost all of which is currently untapped. These resources are often located near major population centers and offer a consistent, predictable resource, making it a good candidate for supplementing U.S. clean power production. The realization of actively tuned WECs, enabled by the data from low-cost, high-quality sources such as Integral's low-cost WaveSpotter, significantly improves the potential for economic viability of this resource.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of November 2016, the Integral team's project has generated one invention disclosure to ARPA-E and one U.S. Patent and Trademark Office (PTO) patent application, with at least three more on the horizon. The Integral team has also presented the scientific underpinnings of this technology at professional conferences. A list of presentations is provided below:

"Wave energy converter effects on wave, current, and sediment circulation: A coupled wave and hydrodynamic model of Santa Cruz, Monterey Bay, CA," C. Jones, G. Chang, and J. Roberts, Ocean Waves Workshop, New Orleans, LA, 2015. [Peer-reviewed conference paper published: "Wave energy converter effects on wave, current, and sediment circulation: A coupled wave and hydrodynamic model of Santa Cruz, Monterey Bay, CA," C. Jones, G. Chang, and J. Roberts, Proceedings of the Ocean Waves Workshop, edited by C. R. Nichols, New Orleans, LA, <http://scholarworks.uno.edu/oceanwaves/2015>.]

Chang, G., Jones, C. A., Roberts, J., Magalen, J., Ruehl, K., & Chartrand, C. (2014, December). Wave energy converter effects on wave propagation: A sensitivity study in Monterey Bay, CA. In AGU Fall Meeting Abstracts (Vol. 1, p. 06).

---

<sup>22</sup> [http://energy.gov/eere/water/marine-and-hydrokinetic-resource-assessment-and-characterization#Wave\\_Resource\\_Assessments](http://energy.gov/eere/water/marine-and-hydrokinetic-resource-assessment-and-characterization#Wave_Resource_Assessments)

# PNEUMATICALLY-ACTUATED PV TRACKING SYSTEM REDUCES COST AND IMPROVES RELIABILITY

Updated: January 17, 2017

<b>PROJECT TITLE:</b> Adaptive Fluidic Solar Collectors
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$4,290,433
<b>PROJECT TEAM:</b> Otherlab Inc. (Lead)
<b>PROJECT TERM:</b> February 2013 – September 2017
<b>PRINCIPAL INVESTIGATOR (PI):</b> Leila Madrone

## TECHNICAL CHALLENGE

Solar is the fastest growing source of energy in the United States. Photovoltaic (PV) power conversion, while possible with fixed-tilt panels, obtains a significant efficiency increase and improves its capacity factor if the panels track the sun as it moves across the sky. However, current tracking systems are mechanically complex, increasing the costs of installation, repair and upkeep. This drives up the upfront and operating costs of the solar plant. Lack of tracker modularity decreases the amount of power obtainable from odd-shaped solar sites. Simple, reliable and modular tracking systems are required to continue driving down the cost of tracked solar generated electricity. Additionally, parabolic trough and tower-based Concentrated Solar Power (CSP) plants would benefit from lower-cost, lower-profile tracking heliostats to reduce the costs of the mirror field and improve overall reliability.

## TECHNICAL OPPORTUNITY

Outdoor mechanical tracking systems have a long history of use for astronomical and telecommunications applications, but these markets are not as price-sensitive as solar energy conversion applications. Until the past few years, the PV module has represented the largest cost component of a deployment and trackers were reserved for only the highest-efficiency (and highest-cost) concentrator cells. As PV module prices have declined while efficiencies have increased significantly over the past decade, commercial and utility-scale solar farms have been increasingly implementing 1-axis tracking systems to provide more annual energy production with over 80% of large-scale PV installations now utilizing trackers. Meanwhile, advances in both the materials and process of mass-manufacturing polymer molded products have allowed production of complex forms and structures at significantly lower costs, and with the ruggedness needed for applications in the challenging conditions of a PV system. As a result, there are technical opportunities to transform the approaches being used for solar tracking.



Figure 1: Otherlab's tracking system at Davis, CA testing site.

## INNOVATION DEMONSTRATION

Otherlab began their project with the goal to disrupt the CSP cost structure by engineering a 2-axis tracking system for a heliostat mirror field, and midway through their project, refocused to the development of single axis trackers for flat-panel PV. They had three technical goals: reduce windload by lowering the tracker height; achieve tracking accuracy needed for tower CSP; and substantially decrease complexity and therefore cost of installing in the field. Their approach to addressing these goals was to develop low-cost fluid (air) based actuators. Their technology approach employs centralized fluidics to actuate the trackers while meeting or beating the tracking accuracy of distributed mechanical motor-based systems. The fluidics approach allows the system to be modular, reducing the costs of site excavation and leveling.

The team made extensive use of physics-based modeling tools to develop their initial designs for the actuation system. Two principal designs were initially explored followed by a downselect after several quarters of modeling, rapid prototyping, and technoeconomic analysis. A pneumatically-actuated antagonistic bellows design (Figure 1) emerged as the most feasible and cost-effective option due to its lower overall mass, lower part count, easier fabrication/configuration, and improved pointing accuracy tolerances. Significantly, the bellows actuators are fabricated with a low-cost, high-throughput manufacturing technique. In 2015 Dupont Performance Polymers joined as a strategic collaborator, advising on material selection and manufacturing utilizing their expertise in long-lifetime, harsh environment applications like automotive and marine. While the team was able to meet their technical milestones for accurate two-axis tracking, the global CSP market entered a downturn. The team pivoted to providing single-axis trackers for the rapidly-growing solar photovoltaics tracker market, allowing further design simplifications.

While the bellows-based drive system represents the core intellectual property developed for Otherlab's tracker technology, developing and demonstrating the supporting systems, their integration with the tracker, and ensuring long-term operation was essential to de-risk the platform as a whole. Tracking subsystems were set up and subjected to harsh environmental testing to ensure reliability over the anticipated 30-year lifetime of a PV plant. The tracking system passed the durability testing including simulated wind and snow loading and harsh-environment cycling. Following several design revisions to the bellows and component-level durability testing, the team implemented a ~6 kW outdoor tracking array in Sebastopol, CA, to acquire outdoor test data on a fully-assembled system. This system has been tracking reliably since August 2015. A second, larger (50kW) tracking array was recently deployed in Davis, CA in July 2016.

## PATHWAY TO ECONOMIC IMPACT

In 2014, Otherlab received an Edison Innovation Award for their work on the pneumatic tracker.

In March 2016 Sunfolding was spun out of Otherlab, Inc. as a separate entity to focus on commercializing the tracking technology. Based on the demonstrated performance of Sunfolding and its technology in their initial two-year project Sunfolding was able to attract supplemental funding from the California Energy Commission (CEC, \$1M) to allow the deployment of ~300 kW of tracked PV in 50 kW phases in Davis, CA (with the first phase completed in July 2016). This project is further solidifying the reliability and durability of the tracking system while incorporating successive design optimizations in each stage to improve the ease of installation and repair in the field.

According to Sunfolding's projections, compared to traditional mechanical trackers, Sunfolding's tracker significantly simplifies installation and reduces costs by eliminating failure modes and reducing routine maintenance locations by 95%, cutting the number of unique components to be installed by two-thirds, improving construction tolerances, and reducing construction crew sizes by 30%. In parallel with its performance testing, Sunfolding has pursued an independent technology assessment of its product and production processes, which is a bankability requirement for most large-scale PV system customers. The first draft of the customer-facing bankability report was completed by the engineering firm DNV GL in August 2016.

In 2016, Sunfolding was selected for a \$2M Department of Energy (DOE) SunShot award to advance the production process to high-volume manufacturing and to drive currently specialized components towards more mass-manufactured solutions. Their 15 employees are located in the United States, as is their manufacturing supply chain. Sunfolding has also received outside financial support from private investors and is preparing to raise a Series A venture capital round in 2017.

Sunfolding is actively bidding on supplying new utility-scale single-axis tracked PV fields as the team continues to build out their ~300 kW pilot plant in Davis, CA. The team has a deployment target of >25 MW in 2017 with a pathway to \$100M in revenue within 3 years.

## LONG-TERM IMPACTS

Since Sunfolding pivoted the project towards a single-axis trackers for the PV market, that market has seen significant growth with 6.7 GW estimated to be installed in 2016, with a >\$10B worldwide market by 2020. Competition has increased with several new companies entering the market, but competitor product offerings are undifferentiated. Sunfolding offers long-term impact in several categories.

**LCOE reduction:** At scale, Sunfolding trackers will allow PV installations to achieve costs as low as \$0.06/kWh by 2020 by lowering the upfront cost over currently available trackers and reducing end-to-end project costs. Preliminary estimates indicate that a solar PV system incorporating Sunfolding's tracker results in a nominal LCOE of 5.32¢/kWh in 2020, a 10% improvement over other trackers and 30% over fixed tilt systems.

**Community Solar:** The Sunfolding tracker will work for sites of any size or shape at a cost that is currently achievable only at larger (100MW+) scale. This opens up new markets for tracking, including agricultural projects and community solar projects that serve residential customers who are otherwise unable to participate in the solar energy economy because they do not own or have access to their own roof.

**Grid Benefits:** When the utility experiences high demand on the grid, trackers still produce considerable power relative to their noontime peak output. Solar production that is available later in the day will mean less air pollution from gas-fired generators during peak periods.

## **INTELLECTUAL PROPERTY**

As of August 2016, the Sunfolding project has generated two U.S. Patent and Trademark Office (PTO) patent applications.

# LOW-POWER MICROSCALE TRACKING FOR LOW-PROFILE DAYLIGHTING

Updated: January 30, 2017

<b>PROJECT TITLE:</b> Self-Tracking Concentrator Photovoltaics
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$3,404,028
<b>PROJECT TEAM:</b> Glint Photonics
<b>PROJECT TERM:</b> April 2013 – March 2017
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Peter Kozodoy

## TECHNICAL CHALLENGE

Artificial lighting accounted for about 10% of total U.S. energy consumption in 2015 (about 9.7 quads). A significant portion of this energy consumption occurs when sunlight is shining directly on the building. Daylighting can offset artificial lighting energy consumption while delivering higher quality, full-spectrum sunlight into interior spaces but typical daylighting options such as windows and skylights can only address areas near the building skin. Tubular skylights and daylight concentrators have been explored to deliver light deeper into buildings. However, it is difficult to provide a steady source of lighting due to the sun's changing position in the sky. Daylight concentrators that require complex mechanical trackers to keep the system pointed at the sun have been expensive and have not achieved significant market penetration. Nearly all currently available daylighting systems require major building modifications to route light pipes, impacting the integrity and aesthetics of the building, as well as driving up installation cost. The introduction of a low cost, low profile, stationary and aesthetically pleasing daylighting system could result in significant reduction in artificial lighting energy use during daylight hours.

## TECHNICAL OPPORTUNITY

Approaches for daylighting concentrator systems have been limited by two major factors. The first is the quality, durability, and cost of the optics and the second is the requirement for a mechanical tracking platform to keep the optics pointed at the sun. Recently, advances in achieving high precision, low cost molded optics have enabled consideration of new optical designs. High clarity, durable, injection molded plastic optics, such as lens arrays, can now substitute for expensive and heavy glass components in many situations. These components are amenable to high volume manufacturing, thereby lowering cost and facilitating the adoption of low-profile optical systems to allow a more aesthetically pleasing appearance. New optical designs allow the external tracking requirements to be shifted to the interior of the panel, allowing for stationary, fixed tilt installation.

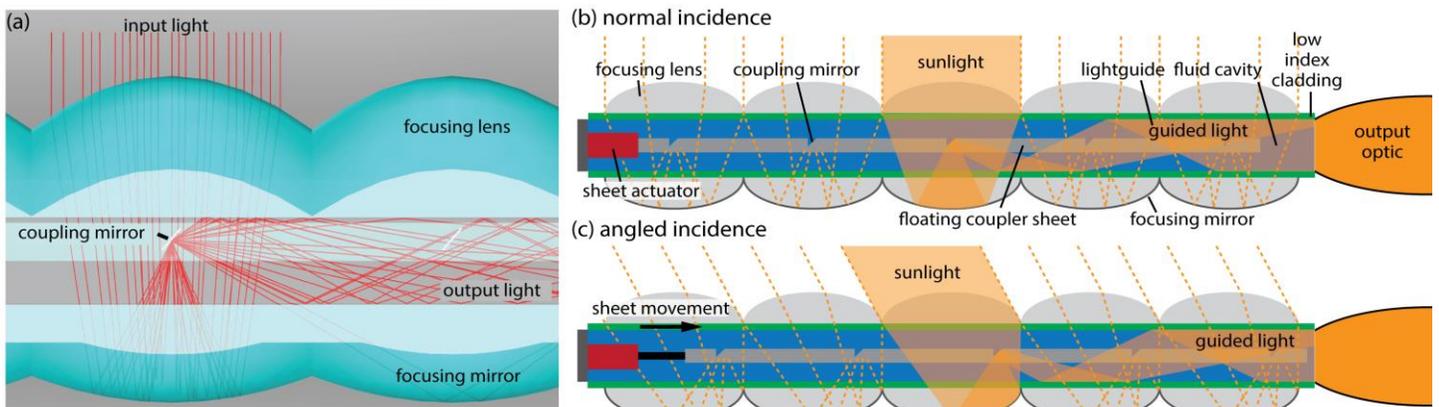
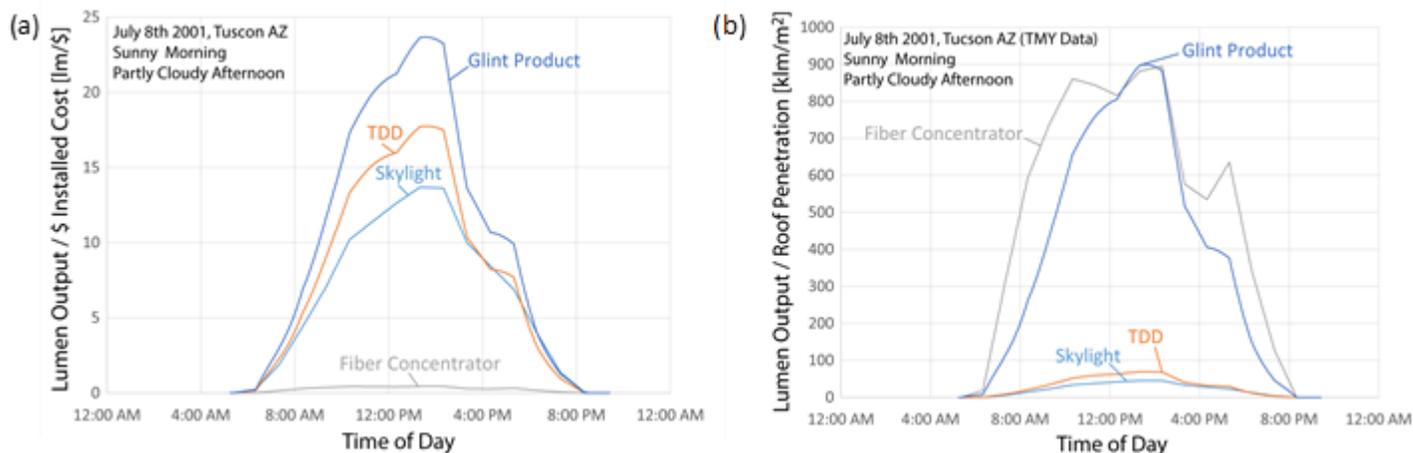


Figure 1: Illustration showing a cross section of the Glint catadioptric optical system. Ray trace shown in (a), tracking action shown in (b). Incoming light is focused onto a light coupling mirror, which passes the light into the lightguide.

## INNOVATION DEMONSTRATION

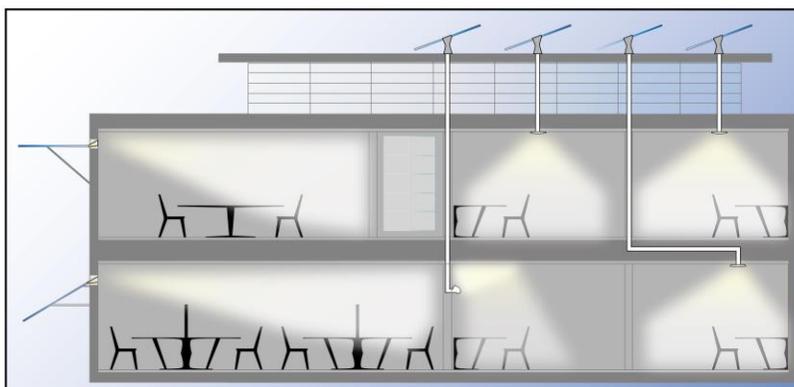
Glint Photonics' (Glint) goal was to improve sunlight capture through a low-profile tracking system using a novel optical design. Furthermore, Glint sought to improve light transfer into the building using a low-cost design that easily integrates into building structures. Glint's original capture design featured a single lens array and a fluidic optical system. However, Glint's modeling and experimental work revealed fundamental limitations in the fluidic optical design. Therefore, Glint redesigned the tracker and settled on a catadioptric optical system (Figure 1) that uses both reflective and refractive optics to access a large range of incident angles up to about 60 degrees off axis.



**Figure 2: Daylighting system output during a representative day in Tucson, AZ (based upon TMY data). Data is shown per installed capital cost (a) and per unit area of roof penetration (b). TDD = Tubular Daylighting Device.**

The catadioptric system uses an active microscale tracking scheme that adjusts the position of an array of reflective optics (the light couplers) at the foci of the reflective back lenses. A closed-loop control system actively adjusts the position of the coupler array throughout the day to follow the sun's movement. Actuation of the coupler sheet is accomplished via magnetic transmission, allowing the actuators themselves to be located outside the panel optics. Glint has demonstrated tracking concentrator prototypes at the 4 inch scale (7x6 lens elements) with optical efficiencies<sup>23</sup> between 30-45% (depending on the angle of incidence) using the company's first generation optical design. The prototype components have been subjected to temperature cycling and UV exposure tests with no appreciable degradation observed (<0.5%/yr degradation in transmission projected). Glint is now developing the next generation panel, which will be 170 in<sup>2</sup> in size with 14x26 lens elements. The new panel is designed to have an output of >18,700 lumens/m<sup>2</sup>, based on improved optics, boosting the optical efficiency to near 50%. The performance and cost effectiveness of the Glint system is expected to surpass that of comparable tubular daylighting devices (TDDs) or fiber based daylighting systems (Figure 2), both in terms of lumens per dollar and light delivered per area of roof penetration.

Glint has also worked on light transmission and delivery methods compatible with low cost, attractive installations (Figure 3). Glint tested several configurations for optimal light transmission and found hollow reflective light pipes to be the most advantageous as they do



**Figure 3: Diagram of rooftop concentrator and façade-mounted panels providing daylight to building interior.**

<sup>23</sup> Optical efficiency is defined as the ratio of the luminous emittance (lumens per unit area) from the concentrating panel (exiting the waveguide) to the luminous energy incident on the aperture of the concentrating panel (illuminance).

not attenuate the transmitted spectrum, have high optical efficiency, and are designed to fit within architectural wall spaces. Its design includes a reflective film applied to inexpensive sheet metal ductwork and can accommodate turns and bends within the wall spaces. Unique among daylighting technologies, the Glint panels can also be façade-mounted as awnings or light shelves (see Figure 3), with output optics that project captured light deep into a building interior at high efficiency.

To date, this on-going project has demonstrated the feasibility of the daylighting system at the component level. The company's innovation was made possible through the coupling of newly available, inexpensive precision molded optics with the Glint's novel optical design. The current techno-economic analysis for the new generation design estimates an installed cost of \$177/ft<sup>2</sup> of concentrator for a typical roof-mount situation. This is comparable to tubular daylighting devices and an order of magnitude less expensive than existing commercial products with trackers.

## PATHWAY TO ECONOMIC IMPACT

Glint has developed a light delivery strategy based on discussions with lighting industry experts who have helped refine and vet the company's design to minimize cost and ensure potential customer concerns would be addressed. The progress made during the ARPA-E award led to a \$1.08M follow-on award from the Building Technologies Office within the Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) in 2016, under which Glint will continue to advance its technology towards a commercial-ready product, fully integrating all components of the light collection and delivery system and optimizing performance. Furthermore, they will be enhancing the durability/reliability of the whole product and validating the performance and installation procedures through active test deployments on buildings. Product introduction to the market will be facilitated by partnering with several contract-manufacturing firms in the U.S. to fabricate and assemble the daylighting system domestically.

## LONG-TERM IMPACTS

Through its work on this project, Glint has pioneered the design and engineering of planar solar tracking systems for low-profile solar capture and concentration. The technical knowledge gained in the project has the potential to facilitate tracked solar light capture for both daylighting and solar energy applications. The potential impact of large-scale daylighting adoption would reduce lighting energy by as much as 70% for high solar irradiance locations in the U.S. (e.g. California and Arizona), and provide 40%-50% savings across the whole country. The global market for daylighting products is projected to be \$6B in 2017, and currently 93% of the market is in skylights for commercial and institutional buildings.<sup>24</sup> The global market for electric lighting is around \$89B, and the segments most easily addressed by Glint's daylighting technology (office, shop, hospitality, and industrial) comprise \$37B of this market.<sup>25</sup> Glint's concentrator has a competitive advantage over alternative systems due to its aesthetically appealing low profile and comparably small-required building penetration area. The concentrator is also adaptable for other optics applications, such as concentrated solar power. For example, in solar PV, low profile and less complex concentration and tracking schemes would enable lower-cost concentrated photovoltaic (CPV) modules.

## INTELLECTUAL PROPERTY

As of January 2017, the Glint project has generated two invention disclosures to ARPA-E and two U.S. Patent and Trademark Office (PTO) patent applications.

---

<sup>24</sup>Lux Research, "Nearly-Zero Energy Building Materials Market to Grow to \$16.5 Billion in 2017," 2013. <http://blog.luxresearchinc.com/blog/2013/06/nearly-zero-energy-buildings-will-deliver-strong-growth-for-materials-manufacturers-but-geographic-segmentation-must-drive-strategy/>

<sup>25</sup>McKinsey and Company, "Lighting the Way," 2013. [https://www.mckinsey.de/files/Lighting\\_the\\_way\\_Perspectives\\_on\\_global\\_lighting\\_market\\_2012.pdf](https://www.mckinsey.de/files/Lighting_the_way_Perspectives_on_global_lighting_market_2012.pdf)

# BUILDING, TRANSPORTATION, AND INDUSTRIAL EFFICIENCY

## Overview:

Improving the energy efficiency of the technologies that keep us comfortable inside buildings, transport us from place to place, or manufacture the materials and goods used in our lives is an obvious way to reduce costs, improve economic competitiveness, save energy and reduce GHG emissions. The challenge is to develop new, energy-efficient devices and processes with competitive performance and cost. ARPA-E has supported a broad range of innovative technologies to improve energy efficiency in the building, transportation, and industrial sectors.

In transportation, the Advanced Management and Protection of Energy Storage Devices, or AMPED program (2012) sought to optimize energy use in electric vehicles through advanced sensing, control, and power management of batteries. The Methane Opportunities for Vehicular Energy, or MOVE program (2012) developed unique ways to store natural gas so that it could be used effectively as a fuel for passenger vehicles. The HEATS program (2010) took a number of innovative approaches toward thermal energy storage and management, including the use of thermal energy to drive heating and cooling of the passenger cabin of an electric vehicle.

Cooling the spaces we live and work in uses about 7.5% of all building energy in the U.S. The Building Energy Efficiency Through Innovative Thermodevices, or BEETIT program (2010) developed a variety of new approaches to lower the energy burden of space cooling. As found in other areas of energy technology, the OPEN solicitations have proven a rich opportunity in the building efficiency space, yielding innovative projects for energy saving window coatings and automated building energy audits. A spinoff from the Strategies for Wide Bandgap, Inexpensive Transistors for Controlling High-Efficiency Systems, or SWITCHES program (2013), which is focused primarily on wide bandgap semiconductor devices for power electronics, has advanced flexible light emitting diodes (LEDs).

The production of pure metals or metal alloys of aluminum or titanium from ore is an enormously energy intensive undertaking, using chemical or electrochemical processes that have not fundamentally changed in decades. The Modern Electro/Thermochemical Advances in Light Metals Systems, or METALS program (2013) is developing innovative new ways to reduce energy consumption and improve productivity in both electrochemical aluminum smelting and thermochemical titanium production. Success in this domain has the additional energy efficiency benefit of promoting the further adoption of these metals in lightweight vehicles and aircrafts.

The examples below provide a good sampling of the energy efficiency portfolio:

- Utah State University (AMPED) – Cell-Level Control in Large Battery Packs
- General Electric (AMPED) – Getting the Best from a Battery
- Otherlab (MOVE) – Intestine-Structured Gas Storage
- United Technology Research Center (MOVE) – Flat, Modular Tank Technology for Natural Gas Vehicles
- Massachusetts Institute of Technology (HEATS) – Advanced Thermal Battery for Climate Control
- University of Texas, Austin (OPEN 2012) – Low Cost Voltage-Controlled Window Can Be Tuned to Block Visible and/or Infrared Light
- University of California, Berkeley (OPEN 2012) – Fast, Automated Building Energy Auditing
- iBeam Materials (SWITCHES) – Low-Cost LEDs on Flexible Metal Tapes
- Alcoa (METALS) – Reimagining Aluminum Manufacturing
- University of Utah (METALS) – A Thermal Pathway to Low Cost Titanium Powder

# CELL-LEVEL CONTROL IN LARGE BATTERY PACKS

Updated: September 27, 2016

<b>PROJECT TITLE:</b> Robust Cell-level Modeling and Control of Large Battery Packs
<b>PROGRAM:</b> Advanced Management and Protection of Energy Storage Devices (AMPED)
<b>AWARD:</b> \$3,968,555
<b>PROJECT TEAM:</b> Utah State University (Lead); University of Colorado, Boulder; University of Colorado, Colorado Springs; National Renewable Energy Laboratory; Ford Motor Company
<b>PROJECT TERM:</b> January 2013 – December 2016
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Regan Zane

## TECHNICAL CHALLENGE

Achieving widespread adoption of hybrid electric and electric vehicles (xEVs) requires minimizing the cost, volume, and weight of the battery while still meeting the range and safety expectations for on-road vehicles. The Department of Energy's U.S. DRIVE initiative has set the goal of a 15-year lifetime at a cost of \$125/kWh with an energy density of at least 235 Wh/kg. These goals are intended to lower barriers to market adoption of electrified transportation for the purpose of ensuring U.S. energy security and reducing greenhouse gas emissions. The cost per kWh has dropped significantly in recent years, and cell-level energy density is now moving above 250 Wh/kg. However, we do not reap the full benefit of these advances: because today's Battery Management Systems (BMS) apply conservative operating limits, the full amount of a battery's energy cannot be accessed. As a result, the battery packs in today's xEVs are typically 1.25 – 2 times larger than would be needed if the full capability of the battery chemistry could be accessed. Developing approaches to cost-effectively maximize cell-level performance remains a significant technical challenge for energy storage systems.

## TECHNICAL OPPORTUNITY

Advances in power electronics hardware and software provide opportunities for significant improvements to the BMS. A key issue in battery management is that the battery packs consist of a string of individual battery cells connected and managed, in series. No two cells within the pack are physically identical due to manufacturing and aging differences, and the circuit configurations used today limit the capacity of a string of cells to the weakest cell in that string. Recent progress in power electronics and adaptive control algorithms present opportunities for battery pack developers to rethink serial cell management.

Specifically, progress surrounding the construction and implementation of low-cost power converters and bypass circuitry has the potential to provide more versatile power architectures for battery pack designers. Such systems will enable the BMS to act on cell-level information, reroute power around weaker cells in a string of cells to optimally deploy the stored energy, and achieve performance gains throughout the life of the battery pack.

## INNOVATION DEMONSTRATION

Under the ARPA-E Advanced Management and Protection of Energy Storage Devices (AMPED) program, Utah State University (USU) and its project partners set out to create a first-of-its-kind advanced cell-level BMS that actively maximizes the performance of each individual cell within a battery pack. The key performance goals for the USU effort were to reduce cell imbalance across the pack by over half, and to extend pack lifetime by 20%.

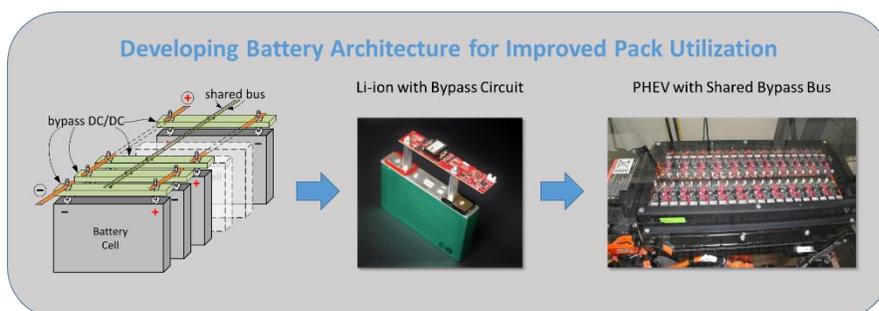


Figure 1: From USU's concept to full pack implementation on a Ford C-Max PHEV pack.

The basis of the team’s concept is their pack electrical architecture, shown in Figure 1, which utilizes a bypass DC-DC converter circuit for each cell in the pack. This circuit topology creates a parallel pathway for current to flow and allows cell-level information to be utilized to optimally deploy each cell’s stored energy. Using this pack architecture, the team developed “active life balancing” so that each cell within the pack reaches the same targeted lifetime. A representative battery pack capacity fade is illustrated in Figure 2 where the spread in capacity between the weakest and strongest cells is indicated by the thin dashed lines. The active life balancing system biases stronger cells to carry more of the electrical load, thus enabling more of the pack’s capacity to be utilized over a greater number of cycles. The desired result is to delay pack end-of-life, the point where the pack cannot supply 75% of rated capacity, indicated by the red and blue triangles in Figure 2.

The major technical challenges that the team faced were in the design and integration of the DC-DC converter boards for a full-scale battery pack. The USU team recognized the opportunity for their novel BMS architecture to do double duty. Their approach combines the BMS with bypass DC-DC converters connected to a 12 V bus, removing the need for a single large DC-DC converter external to the battery pack to power vehicle auxiliary loads. The team’s technoeconomic analysis shows that the new architecture can actually be lower in cost than the baseline approach, even before accounting for the enhanced performance and lifetime of the pack.

The project team has applied their network of bypass converters on a 7.5 kWh Ford Plug-in Hybrid Electric Vehicle (PHEV) demonstration pack. This pack was used to validate their circuit design and assess the value of their active life balancing methodology. During more than one year of accelerated dynamic cycling, the team reduced cell imbalance to half of that presented by the standard passive balancing system, and exceeded the life extension target. While the pack has not reached end of life, the degradation rate for the active life balancing system is projected to yield a 25% increased lifetime.

The team has also worked to evaluate a physics-based cell model to be implemented on their distributed DC-DC converters, to allow model predictive control (MPC). For demonstration, the team has implemented MPC operations on a sub-scale 4-cell battery module, and has shown in simulation that the MPC algorithms can enable an additional 10% increase in cell utilization and an additional 10% increase in lifetime over the baseline active life balancing demonstration without MPC.

## PATHWAY TO ECONOMIC IMPACT

During the ARPA-E project, the USU team worked with strategic partners who can utilize their modular bypass converter architecture in vehicle battery systems, and built an industrial advisory panel of automotive electrical components and sub-systems suppliers. Based on feedback from the industry, the team will next demonstrate a “cost-constrained” power architecture to manage power among small groupings of cells (instead of atop of every cell) while utilizing standard passive balancing circuits within each cell grouping. This system will employ simple rule-based limits to augment standard equivalent circuit control models. An internal development program funded by a major automotive manufacturer has recently launched a demonstration effort for this architecture.

Success on this project could put the bypass converter technology on a path for large-scale deployment on a U.S.-manufactured vehicle early in the next decade. One critical step for deployment of the technology will be reaching sufficient market interest to merit the development of dedicated integrated circuits in a commercial lab. Towards this end, the USU team will continue to build momentum for this technology through Utah State’s recently established Sustainable Electrified Transportation (SELECT) center. The SELECT center is set up to work with industry partners for continued development of the new BMS architecture, and to execute large scale demonstrations that will help develop interest and drive adoption by automakers.

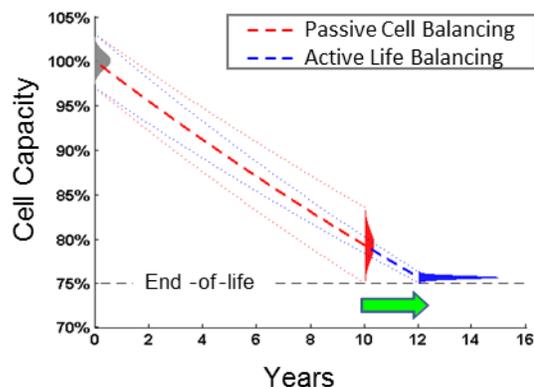


Figure 2: Pack life is dictated by the weakest cell in the pack. Thin dashed lines indicate the spread between the weakest and strongest cells in the battery pack. Red and blue triangles indicate end of useful battery pack life.

The team also continues to explore other application areas. For instance, the Office of Naval Research recently contracted the USU team to apply their advanced cell-level BMS to an energy storage demonstration on a tactical micro-grid, which would enable “plug and play” operation of different energy storage assets on the same electrical bus. Further development of the ARPA-E funded BMS technology for this application is expected to require a distinctly different productization path and set of licensing partners that will continue to leverage the successes of the original ARPA-E award.

## LONG-TERM IMPACTS

The USU team’s technology provides a new mechanism, distinct from and complementary to better utilization of chemistry, to help support market adoption of electric vehicles. Taking the long-term U.S. DRIVE goal of \$125/kWh, the value enabled by 20% improved lifetime and utilization would exceed \$1,000 per vehicle for a 45 kWh EV pack.

The initial on-pack demonstration of this ARPA-E award has established that integrating power electronics into the battery pack can reduce cost, improve usable energy density through better capacity utilization, and improve lifetime for energy storage systems. The project has put this technology on the development path for xEV manufacturers, and the continued development activities for on-vehicle demonstration and manufacturing scale-up that are required before wide deployment.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of August 2016, the USU team’s project has generated two invention disclosures to ARPA-E and from those, derived five U.S. Patent and Trademark Office (PTO) patent applications. The USU team has also published the scientific underpinnings of this technology extensively in the open literature. A list of publications is provided below:

M. Evzelman, M. M. Ur Rehman, K. Hathaway, R. Zane, D. Costinett and D. Maksimovic, "Active Balancing System for Electric Vehicles with Incorporated Low-Voltage Bus," in *IEEE Transactions on Power Electronics*, vol. 31, no. 11, pp. 7887-7895, Nov. 2016.

M. Rehman, F. Zhang, R. Zane, D. Maksimovic, "Advanced cell-level control for extending electric vehicle battery pack lifetime," *Proc. IEEE Energy Conversion Congress and Exposition, ECCE 2016, Milwaukee, WI, Sept. 2016*, pp. 1-8.

M. Rehman, F. Zhang, R. Zane, D. Maksimovic, "Design and control of an integrated BMS/DC-DC system for electric vehicles," *Proc. IEEE Workshop on Control and Modeling for Power Electronics, COMPEL 2016, Trondheim, Norway, June 2016*, pp. 1-8.

Muneeb Ur Rehman, M.; Evzelman, M.; Hathaway, K.; Zane, R.; Plett, G.L.; Smith, K.; Wood, E.; Maksimovic, D., "Modular approach for continuous cell-level balancing to improve performance of large battery packs," in *Energy Conversion Congress and Exposition (ECCE), 2014 IEEE*, pp.4327-4334, 14-18 Sept. 2014.

Muneeb Ur Rehman, M.; Zhang, Fan; Evzelman, Michael; Zane, Regan; Maksimovic, Dragan, "Control of a series-input, parallel-output cell balancing system for electric vehicle battery packs," in *Control and Modeling for Power Electronics (COMPEL), 2015 IEEE 16th Workshop on*, pp.1-7, 12-15 July 2015.

Ryan Jobman, M. Scott Trimboli, and Gregory L. Plett, "Identification of Lithium-Ion Physics-Based Model Parameter Values", *Journal of Energy Challenges and Mechanics*, Vol 2 (2015) issue 2, pp. 45-55.

Stetzel, K., Aldrich, L., Trimboli, M.S., Plett, G., Electrochemical state and internal variables estimation using a reduced-order physics-based model of a lithium-ion cell and an extended Kalman filter, *Journal of Power Sources*, 490-505 (2015).

Wang, Hongjie; Muneeb Ur Rehman, M.; Evzelman, Michael; Zane, Regan, "SIMULINK based hardware-in-the-loop rapid prototyping of an electric vehicle battery balancing controller," in *Control and Modeling for Power Electronics (COMPEL), 2015 IEEE 16th Workshop on*, vol., no., pp.1-6, 12-15 July 2015.

Zhang, Fan; Muneeb Ur Rehman, M.; Wang, Hongjie; Levron, Yoash; Plett, Gregory; Zane, Regan; Maksimovic, Dragan, "State-of-charge estimation based on microcontroller-implemented sigma-point Kalman filter in a modular cell balancing system for Lithium-Ion battery packs," in *Control and Modeling for Power Electronics (COMPEL), 2015 IEEE 16th Workshop on*, pp.1-7, 12-15 July 2015.

Zhang, Fan, M. Muneeb Ur Rehman, Regan Zane, and Dragan Maksimović. "Improved steady-state model of the dual-active-bridge converter." In *Energy Conversion Congress and Exposition (ECCE), 2015 IEEE*, pp. 630-636. IEEE, 2015.

# GETTING THE BEST FROM A BATTERY

Updated: January 30, 2017

<b>PROJECT TITLE:</b> Control Enabling Solutions with Ultrathin Strain and Temperature Sensor System for Reduced Battery Life Cycle Cost
<b>PROGRAM:</b> Advanced Management and Protection of Energy Storage Devices (AMPED)
<b>AWARD:</b> \$3,128,285
<b>PROJECT TEAM:</b> GE Global Research (Lead), University of Michigan, Ford Motor Company
<b>PROJECT TERM:</b> January 2013 – December 2016
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Aaron Knobloch

## TECHNICAL CHALLENGE

The performance and cost per kilowatt hours (kWh) of batteries for electric vehicles (EV) has improved significantly in recent years, and cell-level energy density continues to increase, but we do not reap the full benefit of these advances at the vehicle level because today's Battery Management Systems (BMS) apply conservative operating limits that do not allow the full amount of a battery's energy to be accessed. In fact, the battery packs used in today's xEVs are typically 1.25 – 2 times larger than would be required to power that vehicle if the full capability of the battery chemistry could be accessed. Developing new approaches to battery management that can safely and reliably access more of the stored energy contained in the cells is a key technological challenge for battery systems.

## TECHNICAL OPPORTUNITY

With recent advances in industrial processes and vehicle on-board processing capability, there are two immediate opportunities for enhancing battery management and control. The first is employing sensor technologies that directly probe physical parameters, such as the distribution of temperature and strain across the battery, enabling more informed active and dynamic battery management. Low cost, low-profile sensors are now possible through flexible packaging expertise developed for state-of-the-art, high-volume manufacturing processes used in consumer electronics, integrated circuit (IC) packaging, and miniaturized electronics in healthcare imaging. The second opportunity is leveraging the growing on-board processing capabilities of vehicle control systems to run battery management schemes with control algorithms that can respond dynamically to the sensor information. When more state-relevant information can be measured and battery system developers can utilize real-time models, energy storage systems will realize sizable gains in battery performance. Such opportunities require teams, which bring together experts in sensors, multi-physics modeling and battery system integration.

## INNOVATION DEMONSTRATION

The goal of the GE led research team, in partnership with University of Michigan, and the Ford Motor Company, was to develop a smart, cost effective sensing system that significantly increases the utilization of stored energy in battery packs while maintaining or improving upon system lifetime for vehicle applications. The team addressed three technical challenges – 1) an ultrathin sensor array capable of measuring cell strain and surface temperature across multiple cells within a battery pack, 2) reduced order modeling for real-time computation and observability analysis for a minimum number of

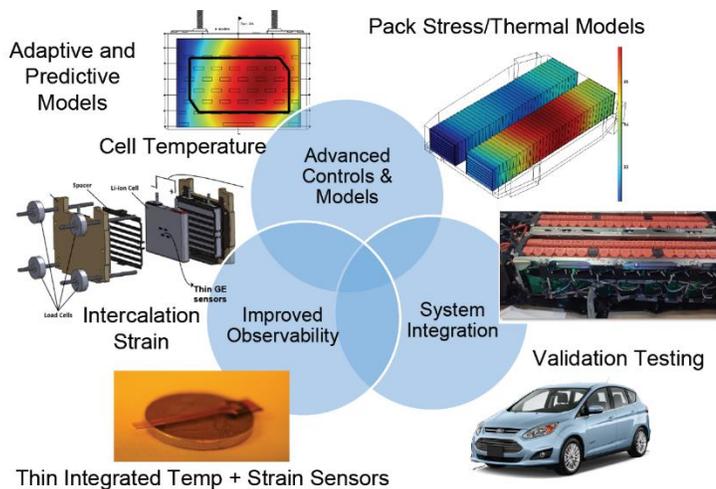


Figure 1: Fusing Physics-Based Models & Sensor Data.

sensors, and 3) sensor-pack integration and system evaluation of sensors and adaptive battery control. The elements of the team's innovative approach are illustrated in Figure 1.

The team evaluated different polymer substrates and different deposited metals for the sensors, with the goal of reducing thickness 20x compared with state of the art battery system sensors, which are typically 2-3 mm thick. The resulting co-located strain and temperature sensor array is under 100  $\mu\text{m}$  thick, enabling the sensor array to be placed between the battery cells within the pack. The sensors achieved accuracy to  $<0.1$  C and  $<0.1$  mm in displacement.

The University of Michigan team developed reduced order physics-based models to utilize the information from the GE sensor array, extracting the thermal and stress features to be used in a new type of battery control algorithm. Predicting the swelling of the entire cell as it charges and discharges in an operating vehicle environment would normally be too computationally intensive for practical use. The team overcame that challenge through observability analysis and estimation techniques that span many physical scales from the electrode level phenomena (5  $\mu\text{m}$ , 50 msec) to the cell level (10 cm, 1 sec), to the pack at the vehicle level (1.0 m, 5 sec). To quantify cell swelling, the team developed innovative experimental methods and specialized laboratory fixtures that measure the battery free and constrained swelling along with its thermal behavior.

The sensor data, paired with a simplified, reduced order physics-based model, are utilized in real-time to optimize pack performance under operation, and make predictions on the state of health of the pack. To evaluate performance, the team instrumented a full battery pack with 76 cells from a Ford Fusion Hybrid Vehicle with their new sensors and control system for testing at Ford Motor Company. The results immediately enabled multiple innovations in real time management. These include setting power limits, fast warm-up, and state of health estimation of capacity fading based on monitoring shifts in bulk stress. Analysis from the team's demonstration on the Ford battery pack indicated that these innovations can enable downsizing of the battery with associated increase in energy utilization by 19% per cell and a projected decrease in available battery capacity of only 0.5% after 100,000 miles of use. The initial testing on a hybrid electric vehicle (HEV) pack was a useful demonstration of this approach to improved battery systems, and the results are promising that the integration of advanced sensors with model-predictive controls can improve performance in EV battery systems, but it will require continued development and deployment on larger battery electric vehicle (BEV) packs to reap the maximum benefits and value from this technology.

## PATHWAY TO ECONOMIC IMPACT

This collaboration brought together a diverse set of experts in sensor technology, materials, mechanics, automotive engineering, controls, and modeling, resulting in advances in hardware and in modeling and control software for battery systems. The IEEE Control Systems Society recognized this team's efforts in pushing the boundary in battery controls with the CSS 2016 Controls Technology Award<sup>26</sup> "for the development of an advanced battery management system accounting for electro-thermo-mechanical phenomena."

Amphenol Advanced Sensors were the commercialization partner for the sensors developed under this program. In December 2013, Amphenol acquired the GE Advanced Sensors business including this research program and the resulting intellectual property. Since the onset of this program, new generation temperature sensors contributed 20% growth in sales for Amphenol Advanced Sensors in EV applications. This growth was a combination of probe, chip on flex, and skin temperature designs.

Based on testing results from the Ford HEV application, the team estimated a potential 15% cost reduction from battery downsizing, and noted improved drivability from faster warm-up in cold weather. That is promising, but for relatively small HEV packs, that savings in the pack would be correspondingly small (measured in the 10's of dollars per vehicle). The advanced sensor and control system would have a larger impact for larger BEV packs, where the utilization improvements that the team demonstrated would yield much bigger savings.

---

<sup>26</sup> The Control Systems Technology Award recognizes outstanding contributions to control systems technology either in design and implementation or in project management.

## LONG-TERM IMPACTS

The GE team sought to improve battery utilization by 20% through the integration of an array of low-cost sensors with an advanced physics-based battery control scheme, and demonstrated 19% improved utilization in validation testing on an HEV pack. Technologies like GE and Michigan's advanced sensors and control offer an additional path to improve effective energy density in a battery pack. Taking the long-term U.S. DRIVE battery cost goal of \$125/kWh, the value for a system-level flexibility enabled by 20% improved utilization would exceed \$1,000 per vehicle for a 45 kWh BEV pack. The pack-level validation testing with Ford during this ARPA-E award demonstrated that battery systems outside of the cells themselves can significantly improve usable energy density through better capacity utilization.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of January 2017, this team's project has generated seven invention disclosures to ARPA-E, five U.S. Patent and Trademark Office (PTO) patent applications, and resulted in four patents.

### Patents:

Youngki Kim, Shankar Mohan, Jason Siegel, Anna Stefanopoulou, "Bulk Force in a Battery Pack and Its Application to State of Charge Estimation," US20160064972A1.

Aaron Knobloch, Jason Karp, Yuri Plotnikov, Chris Kapusta, Yizhen Lin "Battery Cell Health Monitoring using Eddy Current Sensing" US20150340744A1.

Chris Kapusta, Aaron Knobloch, Jason Karp, "Modular Flexible Sensor Array" US20160370210A1.

Chris Kapusta, Yizhen Lin, Jason Karp, Aaron Knobloch, "Method and System for Monitoring Battery Cell Health" US20160160380317A1.

The GE team has also published the scientific underpinnings of this technology extensively in the open literature. A list of publications is provided below:

### Publications:

Ki-Yong Oh, Jason B. Siegel, Lynn Secundo, Sun Ung Kim, Nassim A. Samad, Jiawei Qin, Dych Anderson, Krishna Garikipati, Aaron Knobloch, Bogdan I. Epureanu, Charles W. Monroe, and Anna Stefanopoulou. "[Rate dependence of swelling in lithium-ion cells.](#)" *Journal of Power Sources*, 267(0):197 - 202, 2014.

Shankar Mohan, Youngki Kim, Jason B. Siegel, Nassim A. Samad, and Anna G. Stefanopoulou. "[A phenomenological model of bulk force in a li-ion battery pack and its application to state of charge estimation.](#)" *Journal of the Electrochemical Society*, 161(14):A2222-A2231, 2014.

K.-Y. Oh, N. Samad, Y. Kim, J. Siegel, A. Stefanopoulou, Bogdan I. Epureanu, "A Novel Phenomenological Multi-Physics Model of Li-Ion Battery Cells," *Journal of Power Sources*, Vol. 326, pp 447-458, Sept 2016.

K. Oh, B. I. Epureanu, J. B. Siegel, A. G. Stefanopoulou, "Phenomenological Force and Swelling Models for Rechargeable Lithium-Ion Battery Cells," *Journal of Power Sources*, Vol. 310, pp 118-129, Apr 2016.

N. Samad, Y. Kim, J. B. Siegel, A. Stefanopoulou, "Battery Capacity Fading Estimation Using a Force-Based Incremental Capacity Analysis," *Journal of the Electrochemical Society*, Vol. 163 Issue 8, pp. A1584-A1594, Jan 2016.

Nassim Samad, Boyun Wang, Jason B. Siegel, Anna G. Stefanopoulou, "Parameterization of Battery Electro-Thermal Models Coupled with Finite Element Flow Models for Cooling," *ASME Dynamics Systems Measurements and Control*, to appear 2017.

# INTESTINE-STRUCTURED GAS STORAGE

Updated: October 7, 2016

**PROJECT TITLE:** Safe, Dense, Conformal, Gas Intestine Storage

**PROGRAM:** Methane Opportunities for Vehicular Energy (MOVE)

**AWARD:** \$3,450,000

**PROJECT TEAM:** Otherlab, Inc. (Lead)

**PROJECT TERM:** September 2012 to March 2016

**PRINCIPAL INVESTIGATOR (PI):** Dr. Saul Griffith

## TECHNICAL CHALLENGE

Natural gas vehicles (NGVs) provide an opportunity to increase U.S. energy security by diversifying the resources we rely on for transportation, enabled by the substantial increases in U.S. natural gas reserves and annual production over the past ten years. However, the large, cumbersome, and expensive on-board fuel tanks presently used in NGVs create a major barrier to increased utilization of natural gas as a transportation fuel. Additionally, the low volumetric density of compressed natural gas—26.9% of the volumetric energy density of gasoline—limits the driving range of NGVs and makes cost-effective storage solutions an even more important challenge. Significant improvements must be made to the capacity, conformability, and cost of on-board storage to accelerate NGV adoption.

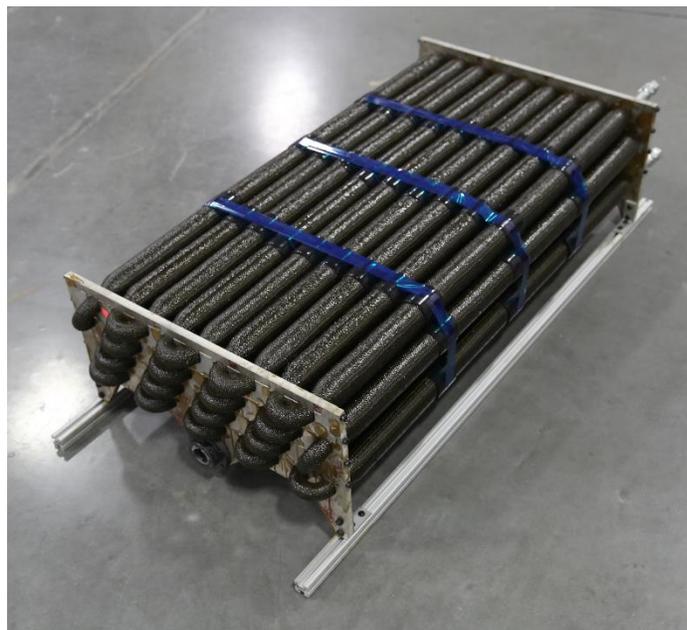
## TECHNICAL OPPORTUNITY

Currently NGVs are outfitted with bulky and expensive cylindrical pressure vessels that can be difficult to fit within the vehicle without compromising passenger or cargo utility. Traditional natural gas storage tanks are cylinders with hemisphere caps. These cylindrical tanks do not always make best use of space within a vehicle, especially when placed in spaces with square or rectangular cross-sections, such as a trunk or truck bed. The technical potential of a conformable gas tank based on innovative geometries, lighter materials and a new overall design presents an opportunity to overcome key market barriers that NGVs currently face. Such a tank could potentially be conformed to a variety of shapes providing higher storage capacity than current cylindrical tanks.

## INNOVATION DEMONSTRATION

To enable low-cost, low-weight fuel storage that conforms to the available space on a vehicle, Otherlab proposed a new natural gas tank design that comprises a single tube with a series of bends that allow the tube to occupy more of a space, much like the bends in an intestine allow it to occupy the space in the abdominal cavity.

Commercial composite tanks for compressed gas storage are made from a plastic liner wound with a carbon fiber and epoxy exterior. However, a wound exterior is not compatible with the Otherlab's proposed bent design. To maintain the required structural integrity needed to safely confine compressed natural gas in a tube with bends, Otherlab developed two innovations: first, fabricating a liner with periodic narrow sections that allow the tank to bend into its final shape, and second, by braiding the exterior of the tank so that the fiber can reinforce both the wide and narrow portions of the tank, as well as the bends.



**Figure 1:** Otherlab's compressed natural gas tank is a folded tube that conforms to the available space, allowing more efficient fuel storage in irregularly-shaped spaces than in a traditional compressed gas cylinder.

Otherlab's space-filling, intestine-inspired design has key advantages over traditional carbon fiber composite cylinders. The conformable tank is well suited to highly automated continuous manufacturing processes, whereas traditional carbon fiber composite cylinders are wound one at a time. Otherlab's design results in a 20% improvement in fuel capacity and driving range when replacing a single, large gas cylinder in a truck bed with a conformable tank that fits into the same rectangular prism storage space. Conformable tanks fit into smaller, more complicated spaces such as a spare tire well, which cannot reasonably accommodate a traditional compressed gas cylinder for fuel storage. By taking advantage of smaller spaces on the vehicle, Otherlab's conformable tank design allows natural gas fuel storage to be moved out of cargo and passenger space, even for a pickup truck with 20 gasoline gallon equivalent (GGE) of natural gas capacity.

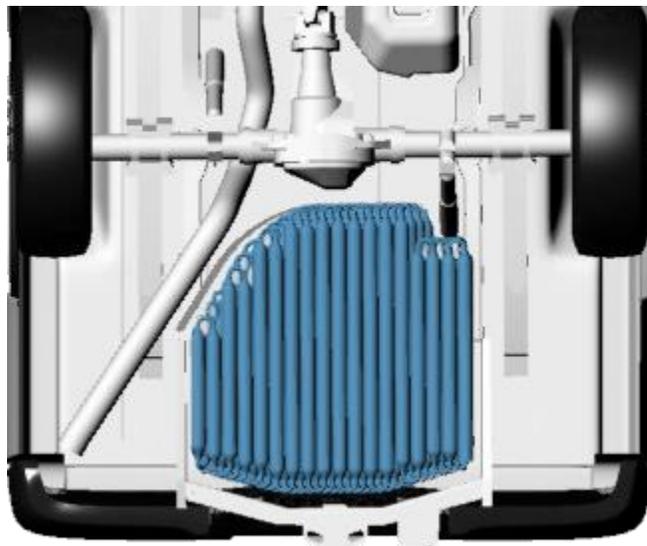


Figure 2: A compressed natural gas tank that conforms the spare tire compartment.

Thus far, the team has fabricated 4 GGE tanks that exceed the target 8100 pounds per square inch (psi) burst pressure target for 3600 psi compressed gas tanks. Otherlab's tanks have a gravimetric energy density similar to other composite tanks, 15 MJ/kg. Otherlab tanks have a volumetric energy density of approximately 5.9 MJ/L of vehicle space compared to 4.75 MJ/L for a cylinder; however, volumetric energy density for both a conformable tank and a cylinder is dependent on the size and shape of the tank enclosure.

## PATHWAY TO ECONOMIC IMPACT

Otherlab formed a new company, Volute, supported by a strategic partnership with Westport Innovations Inc. (now Westport Fuel Systems Inc.), which engineers, manufactures, and supplies alternative fuel systems and components. Volute's initial target application is natural gas pickup trucks and passenger vehicles, which typically carry cylindrical natural gas tanks in the truck bed or trunk, respectively.

Any storage tank technology must be certified to confirm safe performance in automotive conditions before it enters the market. Volute will address this regulatory barrier to market entry for novel tank technologies by contributing to the development and validation of standards applicable to cylindrical and conformable tanks. To that end, Volute has become a member of the CSA NGV 2/HGV 2 Technical Advisory Group (TAG) for compressed natural gas and compressed hydrogen vehicle fuel containers. They have joined this group to address technical issues and draft proposed standards text for industry review, comment, and final approval as an American National Standard. The goal is to develop and approve a new edition of NGV2 that paves a path for the certification of conformable fuel storage tank technologies. The new standards are expected in 2018.

After completing their ARPA-E project, Volute licensed their technology for conformable compressed natural gas storage to Westport. Volute is refining and scaling up their manufacturing process, and has begun a hydrogen storage project.

## LONG-TERM IMPACTS

About 27% of oil consumed in the U.S. is imported, and about 71% of U.S. oil consumption goes to transportation. The U.S. Energy Information Administration (EIA)<sup>27</sup> projects that natural gas use for transportation will reach 710 trillion BTUs by 2040 based on present-day technical factors, compared with the 50 trillion BTUs consumed by natural gas vehicles in 2013. This increase would displace about 300,000 barrels of oil equivalent per day out of the present 12 million barrels of oil equivalent per day of petroleum-based motor fuels.

<sup>27</sup> U.S. Department of Energy, Energy Information Administration, *Annual Energy Outlook 2015*. May, 2015. <http://www.eia.gov/forecasts/archive/aeo15/>

Consumer willingness to adopt NGVs, particularly for light-duty applications, will be increased by technology innovations such as Otherlab's conformable gas tank, which frees up vehicle cargo space and allows vehicles to carry more fuel, and improves range between refueling. Such improved performance may enable further reduction of U.S. dependence on imported oil for transportation needs.

## **INTELLECTUAL PROPERTY**

As of August 2016, the Otherlab team's project has generated five invention disclosures to ARPA-E and five U.S. Patent and Trademark Office (PTO) patent applications.

# FLAT, MODULAR TANK TECHNOLOGY FOR NATURAL GAS VEHICLES

Updated: December 28, 2016

**PROJECT TITLE:** Low Cost Hybrid Materials and Manufacturing for Conformable CNG Tanks

**PROGRAM:** Methane Opportunities for Vehicular Energy (MOVE)

**AWARD:** \$4,299,964

**PROJECT TEAM:** United Technologies Research Center (UTRC) (Lead), Oak Ridge National Laboratory

**PROJECT TERM:** October 2012 – March 2016

**PRINCIPAL INVESTIGATOR (PI):** Dr. Ellen Sun

## TECHNICAL CHALLENGE

The United States is the largest producer of natural gas in the world, increasing its output by more than 50% over the last 10 years, and prices are near historical lows. The potential environmental benefits of this hydrocarbon as a transportation fuel are significant in terms of lower pollutant emissions compared to other fossil fuels. Despite these attractive characteristics, the number of natural gas vehicles in the United States lags far behind other countries in Europe, Asia, and South America. Today, most natural gas vehicles in the U.S. are produced by retrofitting existing gasoline and diesel models, which results in a high purchase premium and the installation of bulky cylindrical compressed natural gas (CNG) tanks that take up essential cargo space. The low volumetric energy density of natural gas also makes it difficult to store sufficient fuel for adequate driving range. Consequently, solutions are needed to make on-board storage of natural gas practical and cost effective so that consumers and businesses can adopt this alternative fuel. Such an approach calls for tanks that can conform more closely to irregularly shaped spaces available on production vehicles.

## TECHNICAL OPPORTUNITY

Cylindrical tanks used today have a conformability factor (the inner tank volume divided by the enclosing outer rectangular cuboid volume) from 60 to 70% (depending on materials). Non-cylindrical designs are challenging due to non-uniform stress distributions, extremely high stress concentrations, and the need for thicker walls and internal supports to address these structural considerations. It is especially difficult to achieve a much higher conformability factor in a tank while also hitting energy density and cost targets acceptable to the market. Recent advances in computer modeling techniques have enabled rapid experimentation with new designs.

## INNOVATION DEMONSTRATION

UTRC designed its tank through an integrated computational optimization, employing detailed topology optimization and structural analysis. The team explored a large design space and conducted trade-off studies to identify key value factors. The design was further simplified by taking inspiration from Plateau's Laws governing intersecting bubbles and considering manufacturing feasibility.

The final design is flat, multi-chambered, and modular, adaptable to the wide range of aspect ratios applicable to different vehicle platforms, as shown in Figure 1. The conformable UTRC design can provide 30% more gas storage in comparison to cylindrical tanks occupying the same space, at a manufacturing cost that is comparable to cylindrical tanks. An individual



Figure 1: Rendering of full-scale tank and illustrations of tank configurations on a variety of vehicles.

tank is composed of two D-shaped chambers on the outer edges, sandwiching a variable number of “stadium”-shaped interior chambers. Domed end caps complete the chambers, and adjacent chambers can be internally connected so that only one external valve is necessary.

UTRC validated the conformable tank design via subscale prototypes. During the course of the project, three parallel paths were taken to fabricate prototypes for design validation and manufacturing process development: (1) steel tank with conventional welding processes, (2) high strength aluminum using solid state welding processes, and (3) long chopped fiber composite using a molding process. The steel prototypes achieved 8,100 psi burst pressure, held for over 70 seconds, and 2,800 pressure cycles, surpassing both the burst and pressure cycle requirements specified by the ARPA-E MOVE program (8,100 psi for 5 seconds; 1,000 pressure cycles). A major achievement with the aluminum tank development was in the area of state-of-the-art solid state welding. High strength aluminum materials are known for difficulty in welding by conventional welding processes. Friction stir welding and linear friction weld processes were developed for aluminum alloy 7055. The chopped carbon fiber polymer matrix composite material and fabrication process were validated using a cylindrical tank, which survived the 8,100 psi burst test.

The team ensured that the manufacturing processes are viable for volume productions. A detailed cost analysis was carried out on the aluminum conformable tank, including raw materials, capital equipment, step-by-step labor and materials, and overhead cost. A \$1,700 volume production cost was projected, well within the current natural gas tank market price range. This cost analysis was reviewed with one major cylinder manufacturer and one automotive OEM. For the composite conformable tank, UTRC collaborated with ORNL on automated manufacturing processes and utilizing low cost carbon fibers.

## **PATHWAY TO ECONOMIC IMPACT**

Under the MOVE project, UTRC has advanced integrated design and optimization methods for complex structural components, and developed manufacturing strategies for lightweight alloys and carbon fiber composites. UTRC is executing a licensing strategy to commercialize its conformable tank technology.

In December 2015, UTRC signed an agreement to license the composite conformable tank technology to Adsorbed Natural Gas Products (ANGP) for composite, non-metal tanks containing activated carbon adsorbents at operating pressures up to 1,000 psi. UTRC is working with a consortium of partners assembled by ANGP to take the technology to commercialization, including a tank fabricator, the manufacturer of a patented activated carbon adsorbent material (enabling low-pressure storage), a supplier of a miniature rotary compressor fuel pump, and an automotive OEM. As of late 2016, UTRC is embarking on a joint development program funded by ANGP to support the certification of the conformable tank under ANSI NGV2-2007 standards for compressed natural gas vehicle fuel containers, a prerequisite to commercialization. This activity is targeted for completion in the second quarter of 2017.

UTRC is also pursuing parallel paths for licensing its technology for high pressure (3,600 psi) CNG applications, and continues to work with automotive OEMs to advance the technology for commercialization.

## **LONG-TERM IMPACTS**

The advanced materials and manufacturing processes developed for the conformable tanks have additional potentially energy-saving applications in other areas such as building systems and aerospace.

The availability of CNG tanks that reduce the space penalty for fuel storage, at cost parity with existing tanks, lowers a significant barrier to adoption of natural gas-powered vehicles. Adoption in light-duty vehicles, which represent over 70% of highway transportation fuel consumption, may occur first for fleet vehicles where a centralized fueling infrastructure can be used. Wider adoption will likely depend on both policy and the relative prices of natural gas and oil.

## **INTELLECTUAL PROPERTY AND PUBLICATIONS**

As of December 2016, the UTRC team’s project has generated 21 invention disclosures to ARPA-E including 11 U.S. Patent and Trademark Office (PTO) patent applications.

# ADVANCED THERMAL BATTERY FOR CLIMATE CONTROL

Updated: January 25, 2017

<b>PROJECT TITLE:</b> Advanced Thermo-Adsorptive Battery Climate Control System
<b>PROGRAM:</b> High Energy Advanced Thermal Storage (HEATS)
<b>AWARD:</b> \$3,556,689
<b>PROJECT TEAM:</b> Massachusetts Institute of Technology (Lead), Northeastern University, University of Texas-Austin, University of California, Berkeley, Ford Motor Company
<b>PROJECT TERM:</b> December 2011 – September 2016
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Evelyn Wang

## TECHNICAL CHALLENGE

Cabin heating and air conditioning play an important role in vehicle energy management. Degradation in efficiency, when running air conditioning, is reflected in the Environmental Protection Agency's shift toward efficiency tests that include hot weather operation. This thermal management issue is particularly acute in electric vehicles (EV) because using electrical energy stored in the traction battery for cabin heating or air conditioning reduces the energy available for vehicle propulsion, thus decreasing EV range for a given electric charge.

A potential solution to address the energy requirements of vehicle climate control is a thermal battery, which stores thermal energy to provide heating or air conditioning to passengers in the vehicle. Historically, thermal batteries have not been able to provide capacity similar to electrically driven vapor compression systems at comparable energy use. It is also difficult to achieve the energy density, form factor, weight, and volume acceptable to automakers. Finally, cost is a significant consideration, as existing air conditioning systems are low cost following many decades of manufacturing experience.

## TECHNICAL OPPORTUNITY

Recent advances in material sciences have made a new generation of thermal batteries possible. There are advanced materials based on zeolites (aluminosilicates) and metal organic frameworks (MOFs) with exceptional potential to adsorb water vapor. Prior state of art for adsorption-based systems was focused on zeolite materials capable of adsorbing vapor of less than 30% of adsorbent weight (wt%). Recent advances in zeolite materials have produced surface areas of more than 1,000 m<sup>2</sup>/g and pore sizes of ~3 nm, enabling 42 wt% water adsorption capacity. MOFs are a newer class of materials and represent the cutting edge of what may be achievable in adsorption materials. Constructed from metal ions/clusters and rigid organic molecular building blocks, MOFs have exceptionally high surface areas of 6,000 to 10,000 m<sup>2</sup>/g, high porosity, and exceptional vapor uptake capacities. These materials could enable a substantial increase in thermal storage capacity and reduction in size and weight.

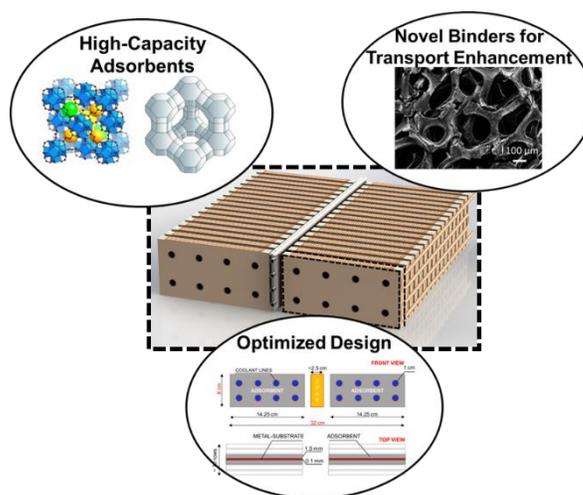


Figure 1: Advanced Thermo-Adsorptive Battery.

## INNOVATION DEMONSTRATION

The MIT team's goal was to develop an advanced thermo-adsorptive battery (ATB) that is both compact (30 liter) and lightweight (<35 kg) for climate control in an EV. The ATB integrates an adsorbent bed (i.e. a vessel containing water vapor adsorbing material) with a condenser, an evaporator, and a water reservoir. When the vehicle is not in use, the ATB can be "charged" by using grid electricity or waste heat to heat the adsorbent bed, which releases water vapor that turns into liquid on condenser surfaces and fills the reservoir. Vapor suction occurs by opening a valve connecting the adsorber to

the evaporator, allowing the adsorber to pull the vapor created over the evaporator's surfaces. When water vapor gets trapped in the adsorbent bed, heat is released and delivered to the vehicle heating, ventilation and air conditioning (HVAC) system for cabin heating. For air conditioning, the system works similarly, except that the bed heat is rejected to the environment, while the cabin heat is removed at the cold source created by the evaporator. The key to success lies in the identification of advanced adsorbent materials and the design and fabrication of the adsorbent bed, as well as the design of the evaporator-condenser unit.

The cornerstone of the project was to define and optimize an adsorbent material commercially viable for an automotive application. The team procured and analyzed existing zeolites and MOFs to set a baseline for water uptake and thermal characteristics to deliver to or remove heat from the cabin to ambient, and structural integrity (for resiliency against vibrations). The team then sought to improve upon the state-of-the-art by synthesizing advanced zeolites and MOFs and characterizing their adsorption rates and capacities. The most promising adsorbents were selected for further cycling and stability testing. While several highly adsorptive new materials were identified, a commercial zeolite was selected for prototype development based on trade-off considerations of its performance, readiness of availability, and cost.

A second key challenge was to fabricate an adsorbent bed that would meet the stringent requirements for the ATB. The bed needed to hold enough adsorbent material to meet thermal capacity, size, and weight requirements, while allowing ease of vapor and glycol flows to preserve heat conduction efficiency. Analysis and experimentation resulted in a copper foam in which the adsorbent material would be poured, layered in between heat spreading fins to carry heat from the binder to the ambient. With continual guidance from Ford, the adsorbent bed was configured into an operational heat pump prototype for testing at the Ford facility.

## PATHWAY TO ECONOMIC IMPACT

Future pathways to impact will be facilitated by demonstrating the ATB prototype performance at Ford. Additionally, EV designers are experimenting with climate control strategies emphasizing more precise delivery of thermal services, such as modular HVAC systems that potentially would have different performance profiles compared to conventional, centrally located systems. The ATB could potentially enhance these alternative climate control designs.

## LONG-TERM IMPACTS

This project could point the way towards expansion of the field of thermally driven climate systems to potentially make EV climate control operate somewhat similar to the conventional internal combustion engine (ICE) driven systems. These longer-term impacts rely upon further investment in fabrication of advanced adsorbents and integration into useful devices. Focusing on completion of an operational prototype, the team opted for commercially viable solutions that could be integrated more easily into the automotive supply chain. The MIT ATB design is flexible and ready to accommodate further advances in materials that will significantly enhance its performance.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of December 2016, the MIT team has generated 12 invention disclosures to ARPA-E and 10 U.S. Patent and Trademark Office (PTO) patent applications. The MIT team has published the scientific underpinnings of this technology extensively in the open literature. A list of publications is provided below:

Ashley, S. Adsorption-based thermal batteries could help boost EV range by 40%, *Automotive Engineering Online*, (8/30/2013) Online [<http://www.sae.org/mags/AEI/12376>]

Furukawa, H., Gandara, F., Zhang, Y. B., Jiang, J., Queen, W. L., Hudson, M. R., & Yaghi, O. M. (2014). Water adsorption in porous metal-organic frameworks and related materials. *Journal of the American Chemical Society*, 136(11), 4369-4381.

Klonowski, P., Goloboy, J.C., Uribe-Romo, F.J., Sun, F.R., Zhu, L.Y., Gandara, F., Wills, C., Errington, R.J., Yaghi, O.M., & Klemperer, W.G. (2014). Di Synthesis and Characterization of the Platinum-Substituted Keggin Anion alpha-H<sub>2</sub>SiPtW<sub>11</sub>O<sub>40</sub>-. *Inorganic Chemistry*, 53(24), 13239-13246.

Narayanan, S., Li, X., Yang, S., McKay, I., Kim, H., & Wang, E. N. (2013, July). Design and optimization of high performance adsorption-based thermal battery. In *ASME 2013 Heat Transfer Summer Conference collocated with the ASME 2013 7th International Conference on Energy Sustainability and the ASME 2013 11th International Conference on Fuel Cell Science, Engineering and Technology* (pp. V001T01A044-V001T01A044). American Society of Mechanical Engineers., Minneapolis, MN [<http://www.asmeconferences.org/ht2013/>]

Narayanan, S., Li, X., Yang, S., Kim, H., Umans, A., McKay, I. S., & Wang, E. N. (2015). Thermal battery for portable climate control. *Applied Energy*, 149, 104-116.

Narayanan, S., Yang, S., Kim, H., & Wang, E.N. (2014). Optimization of adsorption processes for climate control and thermal energy storage. *International Journal of Heat and Mass Transfer*, 77, 288-300.

Yang, S., Kim, H., Narayanan, S., McKay I.S., & Wang, E.N. (2015). Carbon nanomaterials as binders for advanced thermal batteries. *Materials & Design*, 85, 520.

Li, X., Narayanan, S., Michaelis, V.K., Ong, T.-C., Keeler, E.G., Kim, H., McKay, I.S., Griffin, R.G., & Wang, E.N., (2015). Zeolite Y adsorbents with high vapor uptake capacity and robust cycling stability for potential applications in advanced adsorption heat pumps. *Microporous Mesoporous Materials*, 201:151–9.

Yang, S., Huang, X., Chen, G., & Wang, E.N. (2016). Three-Dimensional Graphene Enhanced Heat Conduction of Porous Crystals. *Journal of Porous Materials*, 23, 1647.

Kim, H., Cho, H.J., Narayanan, S., Yang, S., Furukawa, H., Schifres, S., Li, X., Zhang, Y., Jiang, J., Yaghi, O.M., & Wang, E.N. (2016). Characterization of Adsorption Enthalpy of Novel Water-Stable Zeolites and Metal-Organic Frameworks. *Scientific Reports*, 6.

Narayanan S, Kim H, Umans A, Yang S, Li X, Schifres SN, Rao, S.R., McKay, I.S., Rios Perez, C.A., Hidrovo, C.H., & Wang, E.N. (2017). A thermophysical battery for storage-based climate control. *Applied Energy*, 189:31–43.

# LOW COST VOLTAGE-CONTROLLED WINDOW CAN BE TUNED TO BLOCK VISIBLE AND/OR INFRARED LIGHT

Updated: September 23, 2016

<b>PROJECT TITLE:</b> Low Cost Solution Processed Universal Smart Window Coatings
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$4,730,970
<b>PROJECT TEAM:</b> University of Texas, Austin (Lead); Heliotrope, Inc.; Lawrence Berkeley National Laboratory
<b>PROJECT TERM:</b> March 2013 – September 2016
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Delia Milliron

## TECHNICAL CHALLENGE

Each year about 2.5 quads of primary energy is expended for air conditioning to counteract the heat entering through windows from sunlight. Electrochromic (EC) windows, that can be tuned to block light transmission using an applied voltage, are now available commercially as options in sealed double pane window units. However, they have not reached significant market implementation due in large part to high cost, typically around \$50/ft<sup>2</sup>. These windowpanes are typically manufactured via vacuum deposition techniques, and modulate the broad spectrum of sunlight from the visible through the near-infrared (NIR). Realistic operation of these devices in the highest-value applications is expected to save 0.6 quads annually over baseline static windows. In addition to the high cost, a barrier to the use of these windows is the reduction of useful visible light (daylighting) when they are darkened to block heat transmission. Newer technologies are needed that can demonstrate a marked improvement in optical performance, cycling stability, switching speed, and a significant reduction of manufacturing cost to be competitive with inexpensive static coatings (~\$3-5/ft<sup>2</sup> for the coating alone).

## TECHNICAL OPPORTUNITY

Advances in materials science have created new approaches to the fabrication of coating with EC properties. Switching to nanostructured composite EC materials opens up solution-based deposition techniques that could lower the cost of electrochromic window fabrication by about 40% compared to conventional ECs. Furthermore, the recent discovery of a plasmonic EC effect present in some novel nanocomposites allows for independent management of NIR and visible light transmittance. This could enable independent control of visible and IR light carrying heat into building spaces and could save up to an additional 0.1 quads.

## INNOVATION

### DEMONSTRATION

Prior to ARPA-E support, the project team had demonstrated a prototype “dual-band” EC material, able to independently modulate

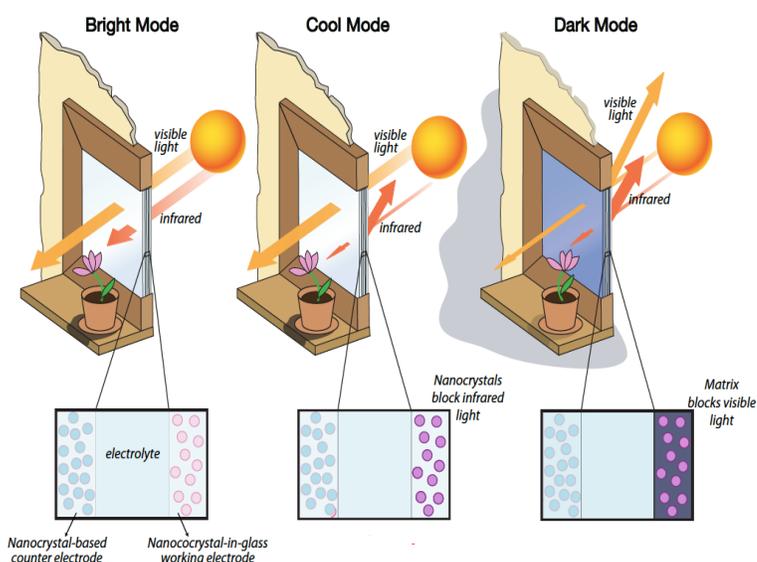


Figure 1: Dual-band electrochromics employing nanocrystals embedded in a polyoxometalate (POM)-derived glass. NIR transmission is modulated via capacitive charging of the plasmonic nanocrystals whereas visible light transmission is independently controlled via polaronic absorption in the glass matrix.

visible and NIR light transmission<sup>28,29</sup>. Early experiments combined indium tin oxide (ITO) nanocrystals within a Nb<sub>2</sub>O<sub>5</sub> polyoxometalate (POM) cluster-derived matrix. The device (Figure 1) could transition to a “cool” state via the application of modestly negative voltages, resulting in a ~65% decrease in NIR transmission ( $T_{\text{NIR}}$ ) while maintaining visible light transmission ( $T_{\text{VIS}}$ ) at ~96%, reducing solar heat gain but allowing daylighting. Applying a more negative voltage decreases the  $T_{\text{VIS}}$ , transitioning the window into a “dark” state much like a traditional EC window. These states are end points on a continuum of optical states accessible via intermediate voltages.

The project goals were to develop devices based on these materials approaches, with improved optical properties, switching speed, and durability. Most significantly, the project focused on scaling up fabrication of devices from 4 cm<sup>2</sup> to 25 cm<sup>2</sup> using a lower-cost, higher-throughput solution-processable technique (such as spray coating) to fabricate all three major components of the device: the electrochromic electrode, the counter electrode, and the electrolyte. The targets for these films included demonstrating +/-5% film uniformity, <15 min switching time, 30%  $T_{\text{NIR}}$  modulation while maintaining  $T_{\text{VIS}}$  at >50%, and cycling the transitions at least 100 times. Accomplishing these challenging targets required rethinking the materials set at the beginning of the project to allow the use of scalable solution-processable techniques.

The team found the maximum achievable  $T_{\text{NIR}}$  with the original ITO/Nb<sub>2</sub>O<sub>5</sub> materials set to be fundamentally limited. They identified a new materials set, CsWO<sub>x</sub>/ITO, and demonstrated substantially improved  $T_{\text{NIR}}$  and  $T_{\text{VIS}}$  values and switching speeds. When coupled with the team’s parallel work on the counter electrode and electrolyte, the EC devices demonstrated performance that surpassed the end-of-project solid-state device targets including the reduced switching time.

Simultaneous efforts at Heliotrope focused on translating the materials and devices to solution-processed manufacturing techniques. The team overcame two significant challenges. First, they were able to reliably charge the devices at the outset via a built-in electrochemical reaction. Second, they were able to fabricate ~100 cm<sup>2</sup> devices with blade coating. It is expected that either this manufacturing technique or curtain coating will readily transfer to a pilot production line or larger.

Having achieved many of the original technical targets, the team began working to ensure durability against UV degradation, long-term cycle life, and reduce the slightly off-neutral coloration observed in some of the states. Mixtures of the tungsten oxide with niobium oxide materials were found to be significantly more color neutral than pure WO<sub>3</sub> or Nb<sub>2</sub>O<sub>5</sub> devices. Further improvements in coloration, switching speed, durability, and spectral transmission of the three states were realized by fabricating a templated mesoscale architecture of WO<sub>x</sub> nanocrystals and infilling the pores with NbO<sub>x</sub>.

## PATHWAY TO ECONOMIC IMPACT

The promise of the project team’s technology has been recognized through investment by Prelude Ventures, receipt of an R&D 100 award in 2013, selection for \$1M in Small Business Innovation Research (SBIR) funding in 2014, and selection for \$250k of funding through the Wells Fargo Innovation Incubator program.

The team is now working on transitioning the the dual-band window technology to a commercial product. The window market is highly sensitive to coloration and requires long-term durability. The team is currently experimenting with variants

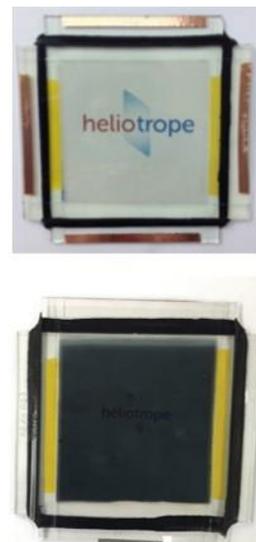


Figure 2: Solution-deposited visible-light-modulating electrochromic prototype in transmitting (top) and blocking (bottom) states.

<sup>28</sup> Nb-Doped Colloidal TiO<sub>2</sub> Nanocrystals with Tunable Infrared Absorption, L. De Trizio, R. Buonsanti, A. M. Schimpf, A. Llordes, D. R. Gamelin, R. Simonutti, and D. J. Milliron, *Chem. Mater.*, 2013, 25, pp 3383–3390

<sup>29</sup> Tunable near-infrared and visible-light transmittance in nanocrystal-in-glass composites, A. Llordés, G. Garcia, J. Gazquez & D. J. Milliron, *Nature* 2013, 500, 323–326

of their successful chemistries to achieve improved coloration and durability, and is also carrying out environmental stress testing to identify and mitigate the deleterious effects of long-term aging.

In parallel, the team is using the new solution-processed techniques to manufacture single-band EC windows that have the potential to be fabricated at a significantly lower cost than incumbent vacuum deposition technologies. The Heliotope team estimates an installed actual selling price significantly less than the ~50/ft<sup>2</sup> for competing products, and a near 7-fold reduction in capital costs for manufacturing equipment. The team has established agreements with window fabricators to produce or sell EC panes rather than competing directly with full insulated glazing unit (IGU) window assembly manufacturers.

The Heliotope team plans to establish itself in the EC window market with a single band product while work continues to improve the coloration, speed, and durability of the dual-band window. The first market for the dual band window may be in higher value "stepping-stone" product offerings such as vehicular windows, skylights, or sunroofs.

## LONG-TERM IMPACTS

The teams work has demonstrated the commercial promise of an entirely new approach to creating controllable window coatings, with a resulting cost reduction that has the potential to enable the projected U.S. energy savings of up to 0.6 quads using electrochromic windows in certain climate areas. Further advances based on this new approach may yield significantly improved control of optical properties with expanded applications and associated further energy savings.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of September 2016, the project has generated three invention disclosures to ARPA-E, three U.S. Patent and Trademark Office (PTO) patent applications and two issued patents:

### Patents:

*"Conductive Transition Metal Oxide Nanostructured Electrochromic Material and Optical Switching Devices Constructed Thereof,"* (2015), Patent No US2015/0277202 A1, T.M. Mattox, B. Koo, G. Garcia, D.J. Milliron, L.De Trizio, C. Dahlman.

*"Nanocrystal polymer composite electrochromic device"* (2015), Patent No US9207513, D.J. Milliron, E.L. Runnerstrom, B.A. Helms, A. Llordes, R. Buonsanti, G. Garcia.

The team has also published the scientific underpinnings of this technology extensively in the open literature.

### Publications:

*"Linear Topology in Amorphous Metal Oxide Electrochromic Networks Obtained via Low-Temperature Solution Processing,"* A. Llordés, Y. Wang, A. Fernandez-Martinez, P. Xiao, T. Lee, A. Poulain, O. Zandi, C.A. Saez Cabezas, G. Henkelman, D.J. Milliron, Nature Materials, 2016.

*"The Interplay of Shape and Crystalline Anisotropies in Plasmonic Semiconductor Nanocrystals,"* J. Kim, A. Agrawal, F. Krieg, A. Bergerud, D.J. Milliron, Nano Letters, 16(6), 3879-3884, 2016.

*"Defect Engineering in Plasmonic Metal Oxide Nanocrystals,"* E.L. Runnerstrom, A. Bergerud, A. Agrawal, R.W. Johns, C.J. Dahlman, A. Singh, S.M. Selbach, D.J. Milliron, Nano Letters, 16, 3390-3398, 2016.

*"Direct Observation of Narrow mid-Infrared Plasmon Linewidths of Single Metal Oxide Nanocrystals,"* R.W. Johns, H.A. Bechtel, E.L. Runnerstrom, A. Agrawal, S.D. Lounis, D.J. Milliron, Nature Communications, 7, 11583, 2016.

*"Switchable Materials for Smart Windows,"* Y. Wang, W. Runnerstrom, D.J. Milliron, Annual Review of Chemical and Biomolecular Engineering, 7, 283-304, 2016.

*"United States energy and CO<sub>2</sub> savings potential from deployment of near-infrared electrochromic window glazings,"* N. DeForest, A. Shehabi, J. O'Donnell, G. Garcia, J. Greenblatt, E. Lee, S. Selkowitz, D.J. Milliron. Building and Environment, 89, 107-117, 2015.

*"Plasmonic Electrochromism of Metal Oxide Nanocrystals,"* A. Llordes, E. Runnerstrom, S. Lounis, D.J. Milliron. Electrochromic Materials and Devices, 363-398, 2015.

*"Nanocomposite architecture for rapid, spectrally-selective electrochromic modulation of solar transmittance,"* J. Kim, G. Ong, Y. Wang, G. LeBlanc, T. Williams, T. Mattox, B. Helms, D.J. Milliron. Nano Letters, 15(8), 5574-5579, 2015.

*"Redox Chemistries and Plasmon Energies of Photodoped In<sub>2</sub>O<sub>3</sub> and Sn-Doped In<sub>2</sub>O<sub>3</sub> (ITO) Nanocrystals,"* A. Schimpf, S. Lounis, E. Runnerstrom, D.J. Milliron, D. Gamelin. Journal of the American Chemical Society, 137(1), 518-524, 2015.

*"Spectroelectrochemical Signatures of Capacitive Charging and Ion Insertion in Doped Anatase Titania Nanocrystals,"* C. Dahlman, Y. Tan, M. Marcus, D.J. Milliron. Journal of the American Chemical Society, 137(28), 9160-9166, 2015.

*"Low Temperature Synthesis and Surface Plasmon Resonance of Colloidal Lanthanum Hexaboride (LaB<sub>6</sub>) Nanocrystals,"* T.M. Mattox, A. Agrawal, D.J. Milliron, *Chemistry of Materials*, 27, 6620-6624, 2015.

*"Nanostructured electrochromic smart windows: traditional materials and NIR-selective plasmonic nanocrystals,"* E. Runnerstrom, A. Llordes, S. Lounis, D. Milliron. *Chemical Communications*, 50, 10555-10572, 2014.

*"NIR-Selective electrochromic heteromaterial frameworks: a platform to understand mesoscale transport phenomena in solid-state electrochemical devices,"* T. Williams, C. Chang, E. Rosen, G. Garcia, E. Runnerstrom, B. Williams, B. Koo, R. Buonsanti, D. Milliron, B. Helms. *Journal of Materials Chemistry C*, 2, 3328-3335, 2014.

*"Influence of Dopant Distribution on the Plasmonic Properties of Indium Tin Oxide Nanocrystals,"* S. Lounis, E. Runnerstrom, A. Bergerud, D. Nordlund, D. Milliron. *Journal of the American Chemical Society*, 136(19), 7110-7116, 2014.

*"Defect Chemistry and Plasmon Physics of Colloidal Metal Oxide Nanocrystals,"* S. Lounis, E. Runnerstrom, A. Llordes, D. Milliron. *The Journal of Physical Chemistry Letters*, 5(9), 1564-1574, 2014.

*"Tunable near-infrared and visible-light transmittance in nanocrystal-in-glass composites,"* A. Llordes, G. Garcia, J. Gazquez, D. Milliron. *Nature*, 500, 323-326, 2013.

*"Regional performance targets for transparent near-infrared switching electrochromic window glazings,"* N. DeForest, A. Shehabi, G. Garcia, J. Greenblatt, E. Masanet, E. Lee, S. Selkowitz, D. Milliron. *Building and Environment*, 61, 160-168, 2013.

# FAST, AUTOMATED BUILDING ENERGY AUDITING

Updated: January 27, 2017

<b>PROJECT TITLE:</b> Rapid Building Energy Modeler - RAPMOD
<b>PROGRAM:</b> OPEN 2012
<b>AWARD:</b> \$2,834,899
<b>PROJECT TEAM:</b> University of California – Berkeley (Lead), Indoor Reality, Baumann Consulting, Lawrence Berkeley National Laboratory (LBNL)
<b>PROJECT TERM:</b> April 2013 – November 2016
<b>PRINCIPAL INVESTIGATOR (PI):</b> Avidesh Zakhor

## TECHNICAL CHALLENGE

Building energy use accounts for ~40% of total U.S. energy consumption (or approximately 39 quads in 2015) and is the largest cost in building operations. As much as 30% of a building’s energy consumption can be lost due to inefficiencies in its operation or its original design. Retrofitting or retro-commissioning buildings for improved energy efficiency, requires determining the most impactful modifications through an energy audit. While retro-commissioning can typically reduce whole building energy consumption by ~16% and pay back in a few years, less than 5% of buildings undergo an audit and retro-commissioning due to the high upfront cost, time, and complexity associated with the auditing process. A fast, automated, accurate, and inexpensive process is needed to rapidly assemble building energy models to recommend the most impactful energy retrofit and recommissioning options to save building energy.

## TECHNICAL OPPORTUNITY

Building energy audits today are performed manually, requiring extensive time (normally several days) to assess the various components of large buildings by a skilled professional, leading to high costs. Subsequent development of building energy models used to simulate the interplay of energy-relevant components to identify problems and predict the impact of retrofits is also a labor-intensive process. Automation of energy auditing and model generation is now possible due to improved sensors, robotics, computational power and image processing. High sensitivity optical sensors are now available that can provide precise information on scanned features, thereby decreasing measurement inaccuracies. Advances in computing power and optical image recognition algorithms can allow rapid sensing and detection on mobile platforms. Techniques to deal with a moving sensor platform, which have been developed for robots and drones, can be adapted for energy audits, but innovation is still needed to deal with navigation in confined or uneven areas, such as closets, utility rooms, and stairwells.

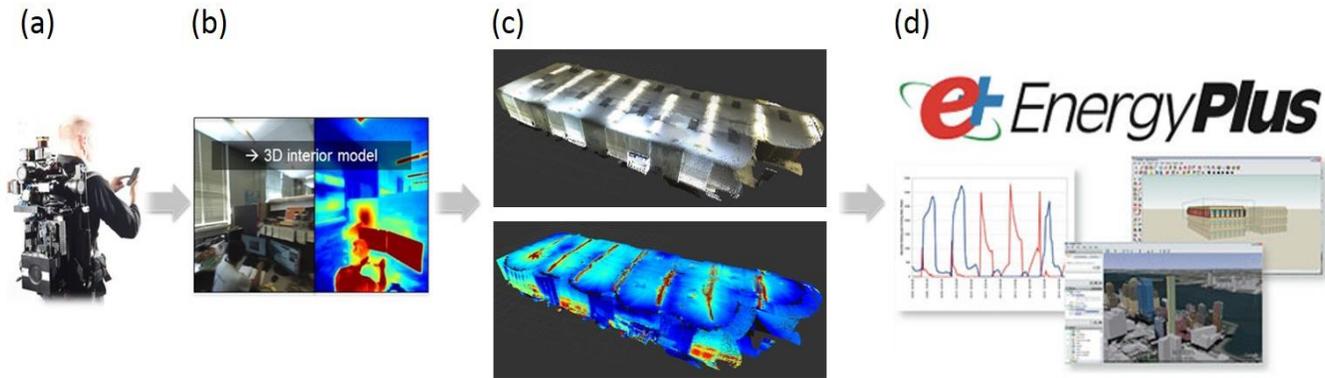
## INNOVATION DEMONSTRATION

The Berkeley team’s goals were to create a human-carried (backpack) audit package, and demonstrate no more than a 10% difference in the predicted energy usage between a manual audit and the backpack audit process in EnergyPlus models for a commercial building with at least 3 floors and a backpack capital cost of <\$40,000. Prior to ARPA-E support, the team at UC Berkeley had demonstrated a set of hardware and software capable of generating crude 3D indoor maps. A wearable backpack-style device had been assembled combining Light Detection and Ranging (LiDAR) scanners, inertial measurement units, and visible light optical cameras to capture data (point clouds) as an operator walked through a building space. The associated software was able to stitch together and render the captured images performing simultaneous localization and mapping (SLAM) while compensating for operator motion/orientation to produce an output that mimics the Google Streetview® type experience for indoor environments.

The project team built on this foundational work by enhancing the accuracy and scalability of the sensor fusion algorithms and integrating the data from added infrared cameras into the SLAM output to allow automated construction of building energy models for use by building auditors. The project team undertook three inter-related technical tasks to address each step of the automatic audit process. The first task was to synchronize the thermal imaging data with the existing SLAM data to assemble visible and infrared (IR) point clouds with improved localization accuracy and scalability. The second task involved improving sensing and detection algorithms with all optical data sets to locate energy-relevant features such as

windows, lighting, and plug loads in the building. The third task was to combine and streamline the SLAM + building element data for easy import into the EnergyPlus building-modeling environment.

The project began with integrating and synchronizing the infrared imaging data with the visible camera data. The team developed optical recognition algorithms to identify key building features and data simplification and translation software to import the results into the EnergyPlus modeling environment. They demonstrated that the system could automatically calculate window to wall ratio, a critical metric for building energy models, within 10% error of that determined via a manual audit.



**Figure 1:** (a) The RAPMOD backpack captures (b) visual and infrared optical data as the operator walks by objects, which is (c) stitched together into 3D point clouds and integrated into building geometry and energy models. The resulting information is streamlined and ported into energy models (d) to recommend energy conservation measures and their impact on building energy use.

The team addressed measurements not well suited to automated detection. Specifically, to determine window U value, the team added a commercial handheld optical scanner that the backpack operator places on building windows to capture the characteristics needed to calculate the U value. The team also addressed the problem of identifying energy consuming components (e.g. HVAC equipment, water heaters, etc.), by using a handheld device (i.e. smartphone) to capture images of large equipment nameplates which are time stamped for synchronization with the location of the backpack. The degree of automated data entry depends on whether the loads are visible or concealed, and whether the load-type has been trained into the recognition algorithms.

After two years, the team demonstrated a backpack audit of a ~69,000 sqft building performed in 1/6 of the time required to complete the same audit manually using established practices. Comparison of total annual building energy consumed in the EnergyPlus models created using the two audit methods showed less than 10% error for the components included in the audit. The cost of the latest version of the backpack is around \$80,000, and the end of project cost target of \$40,000 per backpack appears to be achievable through reductions in the number and sensitivity of sensors incorporated on the backpack.

Continuing work includes streamlining and automating many of the software detection and processing algorithms that remained manually operated. In addition, audit functionality has been developed that incorporates external information about the buildings and allows the operator to dynamically adjust variables within the building model to simulate energy efficiency retrofit/retro-commissioning measures. A client-facing web-based interactive tool has been developed for use on an unlimited number of data sets by the design/construction/audit end-user. The team has also completed testing the audit process in a cold climate region where the heating load is a more crucial factor, with promising early results. Further demonstrations and comparisons are underway in a broader variety of climate zones to refine the energy model processing algorithms and provide assurance of accuracy to potential clients.

## PATHWAY TO ECONOMIC IMPACT

The team at UC Berkeley formed a startup-company, Indoor Reality, to continue development and commercialization of the backpack and associated software built for indoor building mapping. Indoor Reality is targeting the Architecture, Engineering, and Construction (AEC) industry as a first market customer for their building mapping technology. The preparation of accurate as-built documentation is a strong need in the AEC industry, particularly in regions requiring

documentation of energy-relevant performance metrics. The team estimates that ~3.8 billion sqft of building space is affected by benchmarking, transparency, or audit policies. The team plans to employ a service-based business model in which Indoor Reality manages the physical survey and the online documentation and analysis software will be the principal paid product.

In 2016, Indoor Reality completed indoor building scans for approximately 10 customers, has several additional projects booked, and other potential customers in their pipeline. The team has obtained \$200k in follow-on funding from The House Fund, \$500k in seed funding from DPR Construction, and \$345k in angel investments.

## LONG-TERM IMPACTS

The project has made substantial advances in optical recognition technology to achieve precise measurement of building geometry and identify key building elements while ignoring extraneous elements (i.e. furniture). Furthermore, scaling the mapping technology and processing the extremely large amount of data captured as point clouds was a formidable computational challenge overcome by the team. Synthesizing and simplifying data into building dimensions while preserving the needed detail to more accurately model building energy use (compared to today's audit methodologies) represents a significant output of the project.

Building retro-commissioning typically reduces whole building energy consumption by ~16% whereas energy efficiency retrofits can save on average ~45% of building energy. Indoor Reality projects that its products will significantly reduce the cost (by about a factor of 3), time (from days-weeks to hours), and complexity (high to low skill labor) of energy audits, lowering the barrier to entry for many more audit providers, creating jobs in auditing, lowering costs for construction, and ultimately improving U.S. building efficiency.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of January 2017, the project has generated two invention disclosures to ARPA-E. The UC Berkeley team has also published the scientific underpinnings of this technology in the open literature. A list of publications is provided below:

Oreifej, O., Cramer, J., & Zakhor, A. (2014). Automatic generation of 3d thermal maps of building interiors. *ASHRAE Trans.* <http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.645.4516&rep=rep1&type=pdf>

Corso, N. and Zakhor, A. (2013), "Indoor Localization Algorithms for an Ambulatory Human Operated 3D Mobile Mapping System," *Remote Sensing 2013*, vol. 5, no. 12, pp. 6611-6646

# LOW-COST LEDS ON FLEXIBLE METAL TAPES

Updated: January 27, 2017

<b>PROJECT TITLE:</b> Epitaxial GaN on Flexible Metal Tapes for Low-Cost Transistor Devices
<b>PROGRAM:</b> Strategies for Wide Bandgap, Inexpensive Transistors for Controlling High-Efficiency Systems (SWITCHES)
<b>AWARD:</b> \$2,768,468
<b>PROJECT TEAM:</b> iBeam Materials (Lead), Sandia National Laboratory, Los Alamos National Laboratory, University of New Mexico
<b>PROJECT TERM:</b> March 2014 – October 2017
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Vladimir Matias

## TECHNICAL CHALLENGE

Lighting constitutes approximately 10% of the total U.S. electricity consumption. The U.S. Energy Information Administration (EIA) estimates that in 2015, about 404 billion kilowatt-hours (kWh) of electricity were used for lighting in the United States, but most of that energy is wasted as heat. Solid-state lighting (SSL), such as a light-emitting diode (LED) bulb, uses a semiconductor as its light source. Consumer's savings for using SSL are large because SSL uses only a fraction of the electricity of traditional lighting methods and can last far longer. The U.S. Department of Energy estimates that rapid adoption of LED lighting over the next 20 years in the United States could cumulatively save about \$630 billion in energy costs by reducing electricity use by 18.5 trillion kilowatt-hours, equivalent to the output of 100 new power plants. However, despite recent technological advances and rapid decreases in cost, the initial cost of units is still a barrier to wide acceptance.

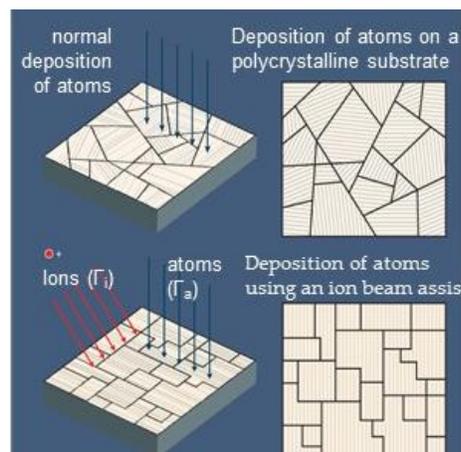
## TECHNICAL OPPORTUNITY

Currently LEDs used for general lighting are manufactured from gallium nitride (GaN) layers deposited on small size, expensive, single-crystal wafer substrates such as sapphire or silicon carbide. This type of manufacturing limits the production of LEDs to discrete chips that need to be diced from the substrate, packaged into a surface mounted device (SMD), and placed in a luminaire (bulb) using costly pick-and-place (P&P) technology. Because many LED applications do not require consistent high quality substrates over large areas, they are potentially amenable to a new manufacturing process using inexpensive substrates in a continuous roll-to-roll (R2R) method. This would also allow elimination of SMDs and P&P, as the LED strips and sheets could be used directly as lighting devices. Replacing the expensive small scale substrate along with considerably simplifying the LED luminaire will help to reduce costs and stimulate wider adoption of LED lighting.

## INNOVATION DEMONSTRATION

The iBeam Materials team's goal is to develop a scalable manufacturing method to produce low-cost (10x reduction) gallium nitride (GaN) LED devices on flexible metal foils for use in solid-state lighting. The fabrication process uses an ion-beam crystal-aligning process (Ion Beam Assisted Deposition, IBAD<sup>30</sup>) to create preferred growth orientations on arbitrary substrates, such as thin, flexible metal foils, which eliminate the need for expensive single-crystal substrates.

The technical goals of this project are to demonstrate a large area LED Light Strip prototype on a 40 x 5 mm flexible metal foil with a luminance of >50,000 candela per square meter (cd/m<sup>2</sup>) or, assuming 3 steradians, 30 lumens, comparable to a typical flashlight. The iBeam team first identified an appropriate metal substrate, molybdenum that can be obtained in thin



**Figure 1: Schematic of IBAD Texturing. Bombardment by ions creates preferred orientations for growth, reducing crystalline mismatch across the substrate.**

<sup>30</sup> Vladimir Matias and Robert H. Hammond, *Surf. Coat. & Tech.* 264, 1 (2015).

sheets or rolls and has a coefficient of thermal expansion matching GaN, which makes it ideal for the IBAD process. They then developed a process called solution deposition planarization (SDP™) to planarize the starting metal substrate over large areas by repeatedly depositing smoothing layers. The SDP layer provides the smoothness needed for the IBAD process and also provides the appropriate base layer for IBAD texturing and a barrier to interdiffusion from the substrate.

After planarization, a buffer layer, typically an oxide layer, is deposited on the metal foil and aligned using an ion beam assisted deposition as illustrated in Figure 1. An initial challenge faced by iBeam was that typical IBAD buffer layer materials have (100) oriented cubic crystal structure with a 4-fold symmetry, which is not compatible with the hexagonal crystal structure of gallium nitride. To overcome this challenge, iBeam developed a (111) orientated buffer layer with 3-fold symmetry to accommodate the hexagonal crystal structure of gallium nitride.

iBeam Materials worked with Sandia National Laboratories to develop a metal-organic chemical vapor deposition (MOCVD) process for depositing epitaxial GaN and other LED device layers on their IBAD templates. They demonstrated gallium nitride growth with dislocation densities of  $\sim 8 \times 10^8/\text{cm}^2$ , comparable to that achieved on single-crystal wafer templates such as sapphire. They then fabricated GaN LED devices directly on their metal-foil supported GaN layers, and demonstrated light emission with no degradation after bending strips to a radius of 7mm. The LEDs fabricated on iBeam's IBAD template exhibited an Internal Quantum Efficiency (IQE)<sup>31</sup>, greater than 70% of the devices fabricated in the same manner on sapphire. The External Quantum Efficiency (EQE), which defines how efficiently the device converts electrons into photons that actually escape from the device and contribute to luminosity, was 13-17% of similar LEDs fabricated on sapphire without any light extraction optimization.

Further work is underway to improve the IQE and EQE of LEDs fabricated on iBeam's IBAD metal substrates. The team is also continuing to improve their IBAD process to reduce cost and improve the performance of LEDs fabricated on the single-crystal-like templates.

The SDP™ and the IBAD processes developed by iBeam are implemented in a continuous R2R deposition, while the GaN MOCVD at Sandia is done in a wafer batch process. Implementing R2R MOCVD for GaN should bring down epiwafer costs by a factor of two, but more cost-effective GaN processes would bring costs down even further. Further significant cost savings are expected from the simplification of the LED packaging since the LEDs come pre-packaged on the metal sheet with the metal substrate acting both as a reflector and heat sink. Contacts and phosphors can be applied using a printing technology.

## PATHWAY TO ECONOMIC IMPACT

The iBeam team has identified a path to market based on the flexible nature of this inorganic LED technology. One of the first-market applications under consideration is horticulture lighting. The iBeam light strip form factor will distribute light with a lower power density and lower heat density than traditional light sources, making it cool enough for leaf contact and enabling an 'intra-canopy' lighting breakthrough product. Ultimately, iBeam sees developing light emitting strips that will enable a cost-competitive LED replacement for the fluorescent light tubes that dominate commercial lighting markets. iBeam's goal is for their light strip to cost less than \$0.1 per kilo Lumens (figure based on iBeam's projections), more than half the cost of conventional LED lighting systems.

The U.S. Department of Energy (DOE), Office of Energy Efficiency & Renewable Energy (EERE) has awarded iBeam funding under the new Small Business Vouchers (SBV) Pilot Program totaling \$225,000. iBeam has also been awarded funding through the New Mexico Small Business Assistance (NMSBA) in the amount of \$20,000 per year for last 3 years for work performed at the National Labs.

The team is developing connections with venture capital investors as a potential pathway to further commercial development. Other applications in display and wearable markets are also being explored.

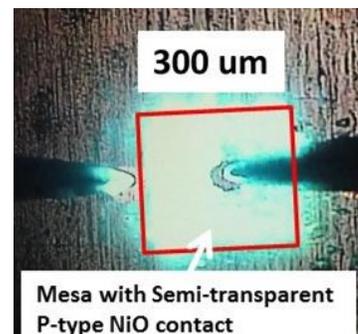


Figure 2: *First-in-the-world* GaN LED device fabricated directly on a metal foil.

<sup>31</sup> the proportion of all recombinations in the active region that produce light

## **LONG-TERM IMPACTS**

SSL offers a great opportunity to reduce electricity consumption, thereby improving domestic energy security and reducing greenhouse emissions. iBeam's goal is for their IBAD technology to lower the cost of LED substrates to as low as \$50/m<sup>2</sup> (current market rate of sapphire substrates is about \$20,000/m<sup>2</sup>) and reduce the cost for luminaire manufacturing using a scalable R2R process eliminating several manufacturing steps. The reduced cost could enable widespread deployment of efficient LED-based solid-state lighting (SSL), and potentially generate sales opportunities outside the U.S.

## **INTELLECTUAL PROPERTY**

The iBeam team's project has generated one U.S. Patent and Trademark Office (PTO) patent application.

# REIMAGINING ALUMINUM MANUFACTURING

Updated: February 6, 2017

<b>PROJECT TITLE:</b> Energy Efficient, High Productivity Aluminum Electrolytic Cell
<b>PROGRAM:</b> Modern Electro/Thermochemical Advances in Light Metals Systems (METALS)
<b>AWARD:</b> \$5,809,354
<b>PROJECT TEAM:</b> Alcoa, Inc.
<b>PROJECT TERM:</b> March 2014 – May 2018
<b>PRINCIPAL INVESTIGATOR (PI):</b> Mark Ripepi

## TECHNICAL CHALLENGE

Reducing automobiles' weight by using more aluminum (Al) and other light metals in their construction is one of the most effective ways to improve fuel efficiency. Therefore, the automotive sector is moving towards the adoption of light metals in their vehicle designs to meet the stringent 2020 and 2025 U.S. fuel economy standards. A prominent example of this being Ford's decision to make extensive use of aluminum in their F-150. However, America's effort to make vehicles that reduce oil imports and increase energy security brings a risk of increasing aluminum imports, because there are few aluminum smelters remaining in America. Due to the high cost of building new plants (>\$2B), and the current low price of aluminum (~\$1,700/ton as of late 2016), retrofitting existing U.S. smelters has the least barriers to increasing U.S. production. Aluminum production is currently performed using the electrolytic Hall-Heroult process, which has seen only incremental improvement since the 19<sup>th</sup> century in making a commodity material. Significant innovation is needed to create a retrofit option for plants using the Hall-Heroult process that reduces cost and energy use, and improves Al production efficiency.

## TECHNICAL OPPORTUNITY

Opportunities to use technical innovation to increase domestic Al production arise from technical advances in other fields. For example, numerous advances have been made in high-temperature materials, especially in the field of electrically conductive ceramics. Likewise, computer modelling techniques developed over the last decade have made it possible to quantitatively evaluate unconventional new cathode designs. Such new designs could enable a retrofit into existing smelting pots, lowering production and energy costs, and potentially making American Al cost-competitive with foreign imports.

## INNOVATION DEMONSTRATION

Globally, the dominant technology employed to make Al is through the Hall-Heroult cell, which electrochemically reduces aluminum oxide dissolved in a molten salt solution at about 950°C. In this cell, the carbon anode is consumed as aluminum metal is formed, creating an ever-changing anode shape with complex changes in salt "crust" formations within the cell as temperatures and current densities change dynamically. In order to maintain production efficiency and prevent electrical shorting, it is important to maintain uniform and close distance between the carbon anode and the molten aluminum that resides on the graphite cathode.

The goal of the Alcoa project is to develop a new technology that allows Hall-Heroult cells to operate with greater reactive surface area within each cell, and to maintain closer and more constant anode-cathode distances without shorting. Alcoa proposed that this could be accomplished by sloping the cathode, and making the cathode surface with TiB<sub>2</sub> plates. This construction material assures greater aluminum wetting than today's cells, and enables a significantly reduced anode-

cathode distance. Alcoa's models show that these changes would reduce energy consumption by more than 20% for a greenfield design using the optimum side angle illustrated in Figure 1c. This greenfield cell design enables a lower anode-cathode distance within the cell and subsequently a reduced energy consumption.

The initial phase of the project focused on the adhesion, corrosion resistance, and wettability of the  $TiB_2$  plates to carbonaceous support materials. High

temperature electrolysis was conducted on materials that had passed a pre-test of high temperature cycling. The electrolysis tests demonstrated the aluminum wettability of the cathode as well as the bonding between the  $TiB_2$  and support structures. A prototype cell was built and multiple tests were performed at 900 A followed by tests at 6,000 A. The 6,000 A cell demonstrated stable operation with an anode-cathode distance, a critical determinant of the energy efficiency, a factor of two to three lower than a standard Hall-Heroult cell. With this performance, modeling showed that an energy consumption of 11.2 kWh/kg can be achieved in a scaled-up, self-heated cell. In addition, the 6,000 A cell demonstrated approximately twice as much output per unit of cell floor area as a conventional cell by operating at a comparable electrode current density but packing in significantly more electrode area due to the sloped design.

To build on this work, Alcoa is proceeding with scale-up to a 65kA self-heated pilot cell to demonstrate the technology at the lowest cost and smallest scale possible that still has direct industrial relevance. This new project phase includes scale-up of the  $TiB_2$  bonding process, developing a process to pre-heat the self-heating cell, and modeling to ensure that a full-sized 200+ kA cell retrofit into a legacy aluminum plant will have improved energy savings using sloped cathode technology. As of November 2016, Alcoa is evaluating the most economical angle of a retrofitted cathode to be used in legacy facilities, and will begin construction of its 65 kA pilot cell early in 2018. Extended operation (30-60 days) is planned to test the self-heated cell including the current efficiency, operation protocols and stability, and energy efficiency.

## PATHWAY TO ECONOMIC IMPACT

Given a successful demonstration of the pilot cell, Alcoa plans to initiate pilot-scale testing and scale-up, drawing on existing infrastructure, to make the technology ready either for internal deployment or for licensing. The commercialization roadmap will require about 5 years of extensive corporate development following the end of the ARPA-E project.

There are two potential paths to market for this technology, greenfield and retrofit applications. Based on Alcoa's techno-economic models, using the sloped cathode design in a greenfield facility would allow for a 5% savings per ton of aluminum produced, comprised of 2/3 in energy consumption and 1/3 savings in increased metal production. This is critical to remain competitive in today's down market for light metals. The capital intensity of this greenfield sloped cathode smelter is estimated to be ~25% less than a greenfield facility of the present best design.

In addition to the benefits of greenfield production, retrofit opportunities represent a significant shorter-term opportunity for commercial impact as well. Alcoa's present total primary aluminum production in the U.S. is ~360k metric tons per year with average energy consumption of 14.5 kWh/kg of aluminum. By retrofitting the sloped cathode technology into Alcoa's existing U.S. smelters, Alcoa primary aluminum production could increase to ~645k metric tons per year with reduced energy use and cost. A retrofit technology developed in the plus-up phase of this sloped cathode project could result in the retention of more than 1,000 direct jobs in the U.S. and many more jobs in the local communities when indirect jobs are considered.

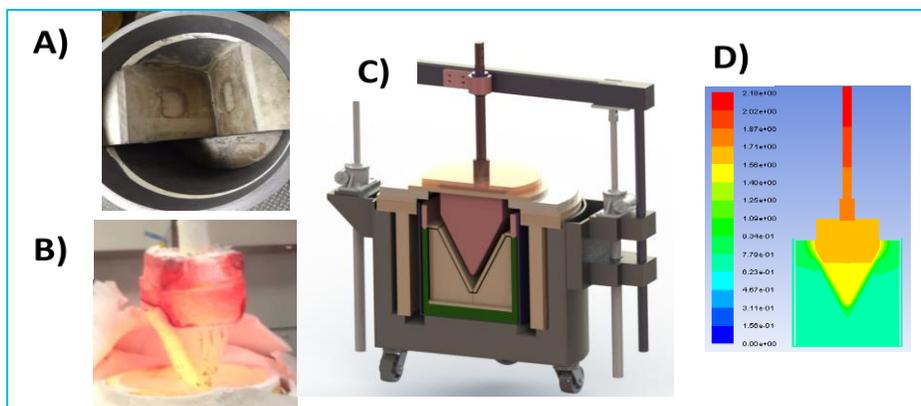


Figure 1: Aspects of Alcoa's original laboratory proof-of-concept 900 Amp cell, including A) bonded cathode plates, B) spent Anode Post-electrolysis extraction, C) design and D) modelling.

## LONG-TERM IMPACTS

The total global market for aluminum is currently 57.9 million metric tons/year (2015 figures), of which 4.5 million is produced in North America<sup>32</sup>. Over the past year, demand for aluminum has leveled off<sup>33</sup>, but there has been consistent year-over-year growth in production (~5.6%) since 2006. Should this trend resume, it would represent an increasing global market size of approximately 3.3 million metric tons of new production per year. A scenario in which Alcoa's sloped cathode technology is utilized in the U.S. to meet even one year's worth of this growing global demand would save 11k GWh per year in energy. This, in combination with switching from coal powered energy sources such as those used in China, would translate to a savings of ~51 million tons of CO<sub>2</sub> per year if hydroelectric energy is used to power the process, or ~27 million tons of CO<sub>2</sub> per year if natural gas were used as the primary electricity generation source. Either scenario would retain existing jobs and create new aluminum production jobs within the U.S. borders.

---

<sup>32</sup> <http://www.world-aluminium.org/statistics>

<sup>33</sup> *ibid*

# A THERMAL PATHWAY TO LOW COST TITANIUM POWDER

Updated: February 6, 2017

<b>PROJECT TITLE:</b> A Novel Chemical Pathway for Ti Production to Drastically Reduce Cost
<b>PROGRAM:</b> Modern Electro/Thermochemical Advances in Light Metals Systems (METALS)
<b>AWARD:</b> \$3,593,494
<b>PROJECT TEAM:</b> University of Utah, Arconic (formerly Alcoa) and Boeing
<b>PROJECT TERM:</b> February 2014 – February 2017
<b>PRINCIPAL INVESTIGATOR (PI):</b> Dr. Z. Zak Fang

## TECHNICAL CHALLENGE

Reducing the weight of vehicles through the use of lightweight metals in place of steel is important for reducing energy consumption and emissions in the transportation sector. Unfortunately, the production of light metals is expensive and energy intensive. For example, titanium (Ti) production via the standard Kroll process consumes 100 kWh/kg, emits 36 kg CO<sub>2</sub>/kg, and results in Ti costs of \$9-10/kg before alloying or processing for parts. As a result, the use of Ti has been limited primarily to aerospace applications with very specific, high-value, performance-critical parts that cannot use other, cheaper metals. Most of the cost and energy intensity associated with Ti production is associated with the difficulty in removing oxygen from the ore, and the subsequent propensity of purified Ti metal to rapidly pick up oxygen and other impurities. In the standard Kroll process, these challenges are addressed by converting Ti ore (an oxide) into TiCl<sub>4</sub>, and then reducing the chloride to Ti metal with Mg. This process is both capital- and energy-intensive, as the Ti metal coming out of the reduction step must be held for over a week under a high temperature vacuum distillation, and the regeneration of Mg from the MgCl<sub>2</sub> by-product is also energy-intensive.

## TECHNICAL OPPORTUNITY

With auto and aircraft manufacturers revisiting all light weighting options to improve fuel efficiency, and with the advent of 3D printing and powder manufacturing techniques for complex parts, there is a large and growing potential market for Ti powder. To meet this demand, a low-energy, cost-effective means is required to produce Ti metal or manufacture Ti parts for high-volume applications. An alternative pathway that avoids chlorination of titanium oxide (TiO<sub>2</sub>) could offer dramatically lower energy input and cost for Ti production, and potentially could expand the use of Ti into higher volume applications.

## INNOVATION DEMONSTRATION

The University of Utah (Utah) project's goal was to develop a novel thermochemical process to extract Ti metal from ore that substantially reduces the cost, energy consumption, and emissions of Ti metal production. Utah's approach uses their new chemical process, which they named "hydrogen assisted magnesiothermic reduction" (HAMR). Mg is always known to be a reducing agent for TiO<sub>2</sub> to Ti metal. However, the equilibrium oxygen content in the Ti metal from Mg reduced TiO<sub>2</sub> is typically higher than 1%, depending on the temperature used, which is unacceptable for industrial applications. This is because Ti-O solid solutions can be more stable than MgO. In order to further reduce the oxygen content in Ti, Utah discovered that Ti-O can be destabilized using hydrogen<sup>34</sup>, making it possible to turn the reduction of TiO<sub>2</sub> with Mg from thermodynamically impossible to thermodynamically favored. This allows TiO<sub>2</sub> to be reduced and de-oxygenated directly by Mg to form TiH<sub>2</sub>, with low oxygen levels that can meet the needs of the industry. TiH<sub>2</sub> can be further processed to Ti metal through industry standard approaches. Utah also developed a two-step technique, which is designed to overcome kinetic barriers and engineering issues. The first step of this technique is the reduction that converts TiO<sub>2</sub> to

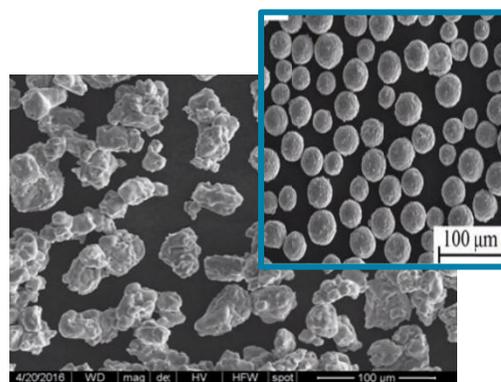
<sup>34</sup>Zhang, Y. Fang, Z. Z., Sun, P., Zhang, T, Xia, Y., et al. (2016). Thermodynamic destabilization of Ti-O solid solution by H<sub>2</sub> and deoxygenation of Ti using Mg. *Journal of the American Chemical Society*, 2016, 138: 6916-6919.

Ti-O solid solutions. The second step is the deoxygenation that refines Ti-O solid solutions to Ti metal with ultra-low oxygen content. The output of the process is HAMR TiH<sub>2</sub> powder, shown in Figure 1. This powder contains a range of particle sizes and shapes, and is suitable for subsequent sintering or other powder applications. The team reliably produced small amounts – 0.2-1 kg of the HAMR TiH<sub>2</sub> powder in a batch and then dehydrogenated it by heating above 400 °C in a vacuum or inert atmosphere to produce commercially pure Ti powder (CP-Ti), and tested its purity against the industry standard for general purpose Ti composition (ASTM B299-13), as shown in Table 1. The HAMR Ti powder produced from the HAMR TiH<sub>2</sub> powder has consistently met the purity requirements defined by the industry standard and the Utah team has developed a reliable recipe for lab-scale production of HAMR Ti powder. A 10 kg batch was produced for further testing at Utah’s commercial partners, Arconic (formerly Alcoa) and Boeing.

	O	C	N	Al*	Fe	Mg	Si
HAMR	0.098	0.009	0.011	0.100	0.045	0.071	0.037
ASTM B299-13	<0.15	<0.03	<0.02	<0.04	<0.15	<0.5	<0.04

**Table 1: HAMR Ti powder composition against industry standard, average of three batches (\*: Al is higher than the standard, however, Ti is almost always alloyed with Al so this is not a concern).**

The deoxygenation process that Utah invented has also enabled a new means to produce high quality spherical powders of Ti and Ti-alloys, a critical and high-value feedstock for additive manufacturing (“3D printing”). Today’s processes to produce spherical powders use plasmas or high temperature gases to atomize a Ti wire or rod. These processes are very expensive (>\$200/kg) because the cost of the Ti wire or rod input is high, and the powder yield is low (only 20-30%, due to the wide distribution of particle size). Using Utah’s new deoxygenation approach, it is now possible to form Ti spheres at about 10’s of micron in size by agglomerating, sintering, and then de-oxygenating smaller Ti particles (a process called Granulation, Sintering, and Deoxygenation, or GSD). GSD can be applied to commercial TiH<sub>2</sub> pigment powder, or to finely ground powder from HAMR or Kroll. GSD can also use recycled Ti alloys as the raw material. Figure 1 contrasts HAMR non-spherical TiH<sub>2</sub> particles vs. GSD spherical Ti-6Al-4V powder. The GSD process produces high quality spherical powder with a nearly monodisperse particle size distribution, suitable to feed a 3D printer.



**Figure 1: Non-spherical HAMR TiH<sub>2</sub> powder vs. spherical GSD powder.**

	Density (g/cc)	O (%)	N (%)	C (%)	Al (%)	V (%)	Fe (%)	Yield (MPa)	UTS (MPa)
GSD	4.419	0.171	0.047	0.075	5.92	4.48	0.33	1059	1105
Commercial powder for Selective Laser Melting (SLM)	4.414	0.204	0.087	0.016	6.38	4.52	0.47	1074	1132
ASTM F2924	--	<0.20	<0.05	<0.08	5.50-6.75	3.50-4.50	<0.30	825	895

**Table 2: GSD powder alloy composition and properties against industry standard and incumbent technology (laser-sintered) (UTS: Ultimate tensile strength).**

The properties of GSD powder relative to the existing industry standard are highlighted in Table 2. To assess the commercial viability of the HAMR process, Utah performed a techno-economic analysis and a full process simulation in ExtendSim (a well-known chemical processing simulation software) to estimate the energy consumption, emissions, and

cost at mass production. The modeling effort included the feed materials, reaction conditions (temperature and pressure), and side processes (pretreatment of the feed materials and post-treatment of the products). As shown in Figure 2, the HAMR process is 50% less energy intensive and generates 30% less emissions than the Kroll process, even after accounting for an additional purification step of the TiO<sub>2</sub> feed prior to the HAMR process. The bulk of the energy and emissions savings comes through eliminating the need to chlorinate TiO<sub>2</sub> to make TiCl<sub>4</sub>, and vacuum distillation after the reduction of TiCl<sub>4</sub>. For the GSD process, the improved yields from this new pathway allows for production to occur at more than 50% lower cost, dramatically lowering the potential price point of high quality Ti powder while keeping energy usage and emissions comparable to the state of practice.

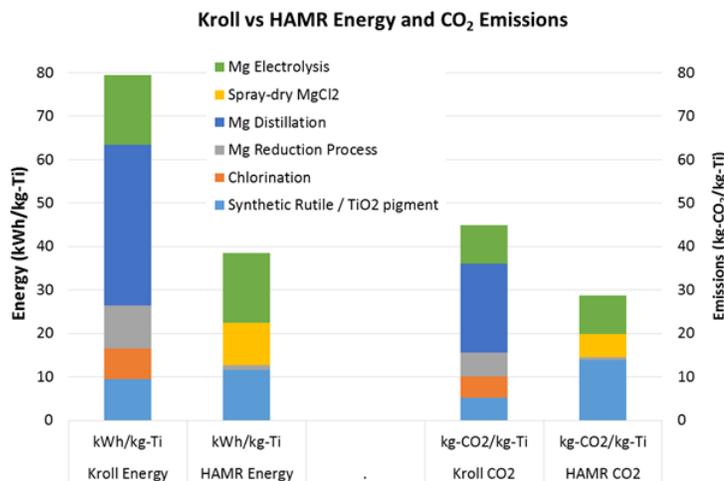


Figure 2: Energy and CO<sub>2</sub> benefits of HAMR vs. Current Ti Production Processes.

## PATHWAY TO ECONOMIC IMPACT

The key challenge for moving forward is scaling up the HAMR and GSD processes from lab-scale demos (~kg batches) to commercial-scale production (thousands or tens of thousands of tons annually). In scale-up there will be many engineering issues in thermal management, reactor design, and system integration that must be overcome and optimized. In addition to obtaining industrial validation of the Ti powders, more samples and parts of much larger sizes must be demonstrated and tested. Utah is working with its partners, Boeing and Arconic, to design new scope and testing protocols that will allow the team to fully scale and validate their products over the next two years. Their goal is to improve their HAMR process for higher volume production of CP-Ti for higher volume markets.

Utah's success with the GSD process for spherical powders offers an ideal first market, with a high-value product for the rapidly growing additive manufacturing industry. The GSD process offers a fast path to scale for this market, and the unique ability to produce custom alloys in small batches for customers to test and improve their 3D printing performance. Utah has spun out a small company, FTP Technologies, to pursue this market. The market size for spherical Ti is expected to reach 2,000 tons in ten years, but faster growth is possible with the lower cost feedstock and improved performance of alloys from the GSD process.

## LONG-TERM IMPACTS

Ultimately, if the HAMR process proves to be scalable, it is projected to reduce the price of Ti parts by 50% or more. It is too soon to determine whether HAMR could drive the price of Ti low enough to displace steel for widespread use in high volume automotive applications, but it does show the promise to dramatically alter the Ti market and increase the range of applications for high performance, lightweight Ti parts. The team projects that its HAMR process could generate billets for automotive and other large-scale use at a scale of around a million tons per year, potentially displacing millions of tons of heavier stainless steel products over time.

## INTELLECTUAL PROPERTY AND PUBLICATIONS

As of December 2016, Utah has generated two invention disclosures to ARPA-E, two U.S. Patent and Trademark Office (PTO) patent applications, and one patent.

### Patents:

Zhigang Zak Fang, Yang Xia, Pei Sun, Ying Zhang. Production of substantially spherical metal powders, US patent 9,421,612 B2.

Utah has also published the scientific underpinnings of this technology extensively in the open literature. A list of publications is provided below:

### Publications:

Zhang, Y., Fang, Z. Z., Xia, Y., Sun, P., Van Devener, B., Free, M., Lefler, H. & Zheng, S. (2017). Hydrogen assisted magnesiothermic reduction of  $\text{TiO}_2$ . *Chemical Engineering Journal*, 308, 299-310.

Sun, P., Fang, Z. Z., Xia, Y., Zhang, Y., & Zhou, C. (2016). A novel method for production of spherical Ti-6Al-4V powder for additive manufacturing. *Powder Technology*, 301, 331-335.

Zhang, Y., Fang, Z. Z., Sun, P., Zhang, T., Xia, Y., Zhou, C., & Huang, Z. (2016). Thermodynamic Destabilization of Ti-O Solid Solution by  $\text{H}_2$  and Deoxygenation of Ti Using Mg. *Journal of the American Chemical Society*, 138(22), 6916-6919.

Zhang, Y., Fang, Z. Z., Xia, Y., Huang, Z., Lefler, H., Zhang, T., Sun, P., Free, M.L. & Guo, J. (2016). A novel chemical pathway for energy efficient production of Ti metal from upgraded titanium slag. *Chemical Engineering Journal*, 286, 517-527.

Cho, J., Roy, S., Sathyapalan, A., Free, M. L., Fang, Z. Z., & Zeng, W. (2016). Purification of reduced upgraded titania slag by iron removal using mild acids. *Hydrometallurgy*, 161, 7-13.

