# TEXAS A&M ENERGY INSTITUTE





Multiscale Models for Seismic Imaging of Fluid Flow





Logistics of Feedstocks for Liquid Fuels



Ocean Renewable Energy Station



A New Wind Turbine





Domestication of Microalgae for Biofuel Feedstock



Nanochannel Confinement of CO<sub>2</sub> in Shale Reservoirs



Mesoscale Interactions in Li-Air Batteries



Water-Energy-Food Nexus



Computer-Aided Design and Discovery of Materials



TEX INS





# The Texas A&M Energy Institute



To address the urgent need for effective, transformative, and sustainable energy solutions requires first the recognition of the importance of all types of natural resources, their proper utilization, and their efficient integration. It also requires the recognition of the important discoveries and advances in materials, catalysis, and separations, as well as fundamental advances in multi-scale energy systems engineering approaches for analysis, simulation, synthesis, and optimization.

At the Texas A&M Energy Institute, we are focused on important scientific and technological energy challenges that impact our society. In tandem, special attention is paid to elucidating the complexity among the interacting components of energy, environment, economics, law, and public policy.

Professor Christodoulos A. Floudas Director, Texas A&M Energy Institute; Erle Nye '59 Chair Professor for Engineering Excellence

In this publication, we highlight 10 proposals that were selected for funding under the Texas A&M Energy Institute's First Proposal Call in January 2015. The objective of this effort was to encourage innovative interdisciplinary energy research collaborations and to support groups of researchers working on important energy-related topics. Each proposal, led by an Energy Institute Faculty Affiliate, received a \$50,000 seed grant and will be part of a competitive group proposal to be submitted to government agencies.

It is our pleasure to support this transformative work, and we hope you enjoy reading more about new frontiers in energy-related research here at Texas A&M University.

#### About the Institute

The Texas A&M Energy Institute pursues and supports new approaches for multi-disciplinary energy research, education, and external partnerships. These approaches cross departmental and college boundaries and address all facets of the energy landscape that naturally connect engineering, sciences, technologies, economics, law, and policy decisions.

The Texas A&M Energy Institute aims to:

- Transform the Energy Research Landscape
- Educate the Next Generation of Leaders in Energy, and
- Establish a Vibrant External Partnerships Program in Energy

#### **Research Themes**

The Texas A&M Energy Institute interdisciplinary research program focuses on the interacting Research Themes of:

THEME 1:	Fossil and Non-Fossil based Technologies for Energy
THEME 2:	Materials, Catalysis, and Separations for Energy

- THEME 3: Multi-scale Energy Systems Engineering
- THEME 4: Energy Economics, Law, Policy, and Societal Impact

#### **Research Areas**

The four interconnected Research Themes are classified into 10 Research Areas:

classified ir	hto 10 Research Areas:	
AREA 1:	Fossil-based Technologies for Energy	
AREA 2:	Renewable Technologies for Energy	
AREA 3:	Geothermal and Hydropower-based Technologies for Energy	
AREA 4:	Nuclear Energy Technologies	
AREA 5:	Energy Storage	
AREA 6:	Energy Efficiency	
AREA 7:	Carbon Capture, Utilization, and Storage	
AREA 8:	Multi-scale Analysis, Simulation, Synthesis, and Optimization of Energy Systems	
AREA 9:	Energy Transmission	
<b>AREA 10:</b>	Energy Policy, Law, Security, and Societal Impact	

<b>ergy</b> ergy	Fossil & Non-Fossil based Technologies for Energy	Materials, Catalysis, & Separations for Energy
act es for Energy	Multi-scale Energy Systems Engineering	Energy Economics, Law, Policy, & Societal Impact

同

# **Transforming the Energy Research Landscape**

#### **Collaborative Effort in Energy Research**

World-class faculty and research teams from multiple disciplines work together and form research collaborations with the best in industry to address the complexity and challenges of important energy problems.

In addition, to enhance the synergy among different disciplines, the Texas A&M Energy Institute introduces annual multi-PI proposal calls and provides seed and matching funds for competitively selected group projects.

#### Texas A&M Energy Institute Faculty Affiliates

More than 220 world-class faculty members and researchers from Texas A&M University System member institutions are Texas A&M Energy Institute Faculty Affiliates. These affiliates are leading experts in the themes, areas, and topics of the Texas A&M Energy Institute's research portfolio.





### A Single-Step Separation and Storage of Methane from Conventional and Unconventional Sources

🕆 Dr. M. M. Faruque Hasan

Assistant Professor, Artie McFerrin Department of Chemical Engineering

As the world looks for cleaner and more sustainable sources of energy for both transportation and electric power generation, fossil fuels continue to be a reliable and cost-effective source. Particularly, natural gas shows the most promise among the fossil fuels for both minimal overall environmental impact and extent of availability.

Methane is the predominant component of natural gas, the major component of shale gas, and it can also be retrieved as



Dr. M. M. Faruque Hasan Assistant Professor Artie McFerrin Department of Chemical Engineering



Associate Professor Artie McFerrin Department of Chemical Engineering



Assistant Professor Artie McFerrin Department of Chemical Engineering



landfill gas, biogas, coalbed methane, and stranded natural gas.

The overall production, storage, and transportation of methane, however, is a critical technology issue. In order to efficiently prepare, produce, and transport methane, it must be separated from impurities like carbon dioxide ( $CO_2$ ), nitrogen ( $N_2$ ), hydrogen sulfide ( $H_2S$ ), and other gases. Due to the presence of these contaminants and their high separation cost, more than 10% of the total U.S. natural gas reserves and numerous coalbed methane, landfill gas and biogas sources are currently not economically viable to produce.

The expensive cost of separation is tied to two major issues: the energy consumed in the separation process and extensive resources for processing. Additionally, once the methane is separated, it must be stored for consumption or transport. Because separation and storage technologies have a history of independent development, energy is often expended twice: during the regeneration of materials for separation and during compression for storage. For stranded gas sources, isolated landfills, or even unconventional gas fields, infrastructure and transport avenues may not exist at all.

A solution to this problem could exist in a new way of tackling this issue: the Plug and Store method. This new method, conceived by Dr. M. M. Faruque Hasan, an assistant professor in the Artie McFerrin Department of Chemical Engineering,



(L-R) Faruque Hasan; Shachit Iyer, a Ph.D. student in Hasan's group; Ishan Bajaj, a Ph.D. student in Hasan's group. Iyer and Bajaj are working on developing theoretical, algorithmic and computational tools to enable the proposed combined separation and storage technology.

and his research group, involves the integration of the methane separation process with the storage process. Hasan will simultaneously separate and store methane in the same vessel and use that vessel to transport the methane for processing, thereby eliminating the need for a separate purification step. He aims to intensify the process through using advanced materials such as metal-organic frameworks (MOFs), a class of nanoporous crystalline materials that exhibit both selectivity and capacity for methane. These MOFs may be able to address, or even resolve this problem.

For many years, scientists have been using MOFs to independently demonstrate both selective separation and storage capabilities. The inherent ultrahigh surface areas and numerous structural possibilities that are possible with MOFs have resulted in significant research on microporous materials.

However, two major challenges remain. First, materials with high selectivity for separation often do not have high-deliverable capacity for storage, and second, materials with high-deliverable capacity for storage often do not have high selectivity for separation. The challenge that Hasan will address is the identification or development of a MOF material with a high ability and high readiness to store methane, but also a material that does not store - but instead filters out-undesirable impurities. This is particularly challenging, since methane typically adsorbs less onto microporous materials than  $CO_9$ .

He and his group will design and optimize a process that will take mixtures of contaminated methane and pass them through an empty vessel packed with an MOF-based adsorbent, and then vent the purge gas – primarily the contaminants – at the opposite





end. Hasan will work to minimize the steps in the process, perhaps even maintaining the same pressure that the gas is under as it comes from the well. For each of the gas mixtures, he will identify the optimal process and the timing to minimize the overall cost of methane production, storage, and transportation, including the entire process from the well to the transport vehicle or power plants.

As an essential component of the analysis, Hasan and his collaborators are considering MOFs, which will enhance the process performance. Unfortunately, the most suitable MOFs for a future separation and storage technology are most likely unknown at this time. Hasan will use a multi-scale screening method to find the MOFs that will purify and store methane in the most energy-efficient and cost-effective manner. Process optimization will be introduced to generate a rank-ordered list of MOFs based on the total cost of separation and storage.

This research will ideally identify the best materials to address the problem, design the optimum process for separation and storage, and identify the least expensive route of implementation, factoring in the initial investments, operating costs, and the cost of materials.

If successful, this single-step separation and storage route will clear a path for easier access to a cleaner alternative to liquid transportation fuels, minimize energy-intensive separation processes, and secure low-cost and sustainable energy for the future.



# **Production/Logistics/Processing Design for the Use of Agricultural Feedstocks for Liquid Fuel Production: Case Studies in Two Regions**

or: Dr. Bruce A. McCarl

Distinguished Professor of Agricultural Economics, Department of Agricultural Economics

According to the Renewable Fuel Standard in the U.S. Energy Independence and Security Act of 2007 – also known as the 2007 energy bill, the United States is required to produce 16 billion gallons of cellulosic biofuel per year by 2022.

The term "cellulosic biofuel" refers to renewable fuel derived from any cellulose, hemicellulose, or lignin that is derived from renewable biomass. More specifically, feedstocks for producing this biofuel include nonfood-based sources like grasses, agricultural crop residues, logging residues, and sawdust.



Dr. Bruce A. McCarl



Dr. Neil Geismar Associate Professor and Mays Research Fellow



Dr. Steve Searcy Professor and Department Head Department of Biological and Agricultural Engineering

In 2013, according to the EPA, the U.S. produced 0.51 million gallons of cellulosic biofuel. Furthermore, the Renewable Fuels Association indicates commercial plants were opened in 2014-2015 that have 75 million gallons of capacity.

Scaling up production of cellulosic biofuels will require solutions to significant logistics and processing challenges. The movement of large volumes of feedstocks, including their water content, will require numerous trucks utilizing rural roads and bridges, additional rail and barge services, and other burdens on infrastructure.

Raw or unprocessed feedstocks will require large areas for storage plus exhibit wide seasonal fluctuation in availability – and most feedstocks are subject to perishability with time and weather conditions. These forces can lead to formidable issues for road and bridge planning, materials handling and facility requirements. Studies have revealed that logistics costs can represent up to one-third of the cost of producing fuels.

With careful design and planning, improving logistics for the production of cellulosic biofuels could greatly

lower the cost of producing cellulosic biofuels, possibly leading to the development of low cost domestic liquid fuel supplies. Cost saving benefits could be found through advancements and developments in storage, densification, and multi feedstock processing technologies.

Traditionally, the processing of feedstocks has taken place in close proximity to the growing or generating location. It is possible that

distributed "hubs" of processing and storage could lead to greater efficiencies, and therefore, lower costs all the way to the consumer. It might also be possible to balance the supply in a particular area of variably available feedstocks with a feedstock supply of more consistency.



A biomass baler is used to collect harvested crops for storage and transportation.

Dr. Bruce A. McCarl, a Distinguished Professor of Agricultural Economics, is leading a team of engineers and supply chain experts that will prepare two case studies on a broad range of logistics issues related to cellulosic biofuel production. They will address the elements of feedstock logistics and the costs involved with location of production, densification, hauling, storage volume, storage loss, moisture, depots, feedstock diversification, and moisture management.

The study will begin with the development of a listing of the





costs of major logistic alternatives to common practices, the potential benefits of adding densification and depots to the process, calculating storage losses and the cost of moisture, as well as the value of diversifying feedstocks. They will also develop a thorough justification of work with comparative budgeting across some simple alternatives and will conceptualize a model to handle diverse alternative logistical, production, and processing scenarios.

Two regions were chosen for the case studies based on the potential availability of feedstocks, as well as switchgrass growing conditions. Both offer feedstocks and lands that are not directly competitive with conventional food crop production.

The first case study area will be a Midwest location – perhaps Indiana – on switchgrass, corn stalks, and wood. The Midwest has existing ethanol production infrastructure as well as a considerable corn residue supply. Additionally, parts of Indiana have substantial areas of marginal lands and stands of trees.

The second case study area will be a southern location in East Texas, focusing on switchgrass and forest products and byproducts. East Texas is in close proximity to large liquid fuels processing facilities that provide supporting infrastructure. Additionally, East Texas has a steady supply of water for production as well as marginal lands and trees. The southern region provides an opportunity to explore longer-duration harvest and storage options because of milder winters.

Both studies will provide a regional analysis and associated modeling to investigate the development of a supply chain,



A tractor pulls a MacDon mower-conditioner through a field as it cuts switchgrass.

plant location, and spatial feedstock production, storage, and densification. The analysis will consider locations of single or multiple feedstock production in addition to biorefinery operation and feedstock movement, storage, and densification. Finally, the research will factor in regional implications for income, greenhouse gas emissions, energy use, and a wide range of energy production costs.





# **Energy Development under Water Scarcity and Climate Change:** A Case Study in the San Antonio, TX Region

Dr. Rabi H. Mohtar

TEES Endowed Professor, Department of Biological & Agricultural Engineering

The availability of water and access to water has dictated civilizations' choices throughout human history. Historically, primary sources of water came through rainfall and surface water; while in the modern era, technology has provided opportunities to exploit underground water sources for use in irrigation, consumption, and industry. The availability of water dictates the viability of food resources and supports food production on large scales. In addition to food, water is intricately intertwined with the production, transportation, and use of most forms of energy, including shale oil and gas.



ice A. McCar

Looking to the future, climate change will impact water resources through anticipated shifts in the patterns of rainfall and water availability. Such a change has the potential to significantly impact competition for water, particularly in the Southwest United States.

#### The Water-Energy-Food Nexus

To better manage our resources, we must gain a more complete understanding of the interdependence between water, energy, and food. Known as water-energy-food (WEF) nexus, a mastery of the relationships between these resources has the potential to strategically inform policy and planning, protect regions from vulnerability, and provide solutions for problems that currently exist or may arise.

The WEF nexus is complex, and there are many variables that are difficult to predict. Existing studies have looked at the role and impact of the WEF nexus on the development of energy, land use, urban growth, and water policies, but few explore the tradeoffs and synergies at regional or national levels, and there has been little consideration for the nexus and the impact of climate variability on water supplies.

Dr. Rabi H. Mohtar, a TEES Endowed Professor in the Departments of Biological & Agricultural Engineering and Civil Engineering, along with Dr. Bruce A. McCarl, a Distinguished Professor of Agricultural Economics, will address these challenges in a new case study in the San Antonio, Texas region. Focusing on understanding the WEF nexus in the context of population growth, climate change, and developing scientific breakthroughs, the pair will address the interrelations of water, food, and energy, and the potential benefits for regional planning and coordination.

#### **Selecting the Region**

Mohtar and McCarl selected the San Antonio region based on the following:

- 1) Increased use of hydraulic fracturing for regional shale oil and gas plays
- 2) Rapid population growth
- 3) Active irrigated food production sector
- 4) Important regional environmental issues, including the emerging water deficit

These four factors highlight the impact that water, energy, and food will have on this area in the future and emphasize the need for the development of a regional WEF plan. Increases in usage of one resource often also affect another resource's availability, leading to compounding challenges. The San Antonio region provides a comprehensive set of these compounding challenges and will add depth to Mohtar and McCarl's analysis.

#### San Antonio Regional Compounding Challenges

- **Challenge: Using More Water Requires More Energy** Oil and gas production from hydraulic fracturing in Texas requires between 10,000 to 30,000 cubic meters of water per well. This process generates large amounts of contaminated water after injection, and challenging decisions must be made about its disposal, treatment, and reuse. Through the entire process, from water collection, transportation to the site, injection, recovery, and treatment and disposal, energy is consumed.
- **Challenge: Using Water Faster than Aquifer Recharge** The Eagle Ford Shale, just south of Bexar County in the San Antonio region, has substantial hydraulic fracturing activity. This area has seen an increase in activity over the last few years and that is expected to continue into the future. Not only does hydraulic fracturing require large amounts of water, but research has also shown that groundwater consumption for oil and gas production can be 2.5 times greater than the rate of recharge in the aquifers. Over time, this demand for water could lead to a decline in the quantity of water available for other uses.
- **Challenge: Using More Energy to Retrieve More Water** A 40% deficit in water is projected for the San Antonio Region, without considering the usage for hydraulic fracturing. The city of San Antonio aims to reduce its reliance on the Edwards Aquifer and diversify its water



portfolio to meet demands of growing agricultural, industrial, municipal, ecological, and recreational uses. In the next 25 years, the city expects to launch brackish ground water desalinization, pump additional water from the Edwards Aquifer, and transport Carrizo Aquifer groundwater into San Antonio. Energy intensive water plans, such as desalinization, will further increase the demand for energy, making critical a clear understanding of the best energy-water portfolio options for the intended development.

#### San Antonio Regional Opportunities

Opportunities do exist in the region for synergistic cooperation – even among diminishing resources.

**Opportunity: Geothermal Energy Generation** 

In many areas in Texas, unique geothermal resources exist in large, exploitable shale formations. More than 12 billion barrels of water are produced each year from crude oil and natural gas wells. This water, often extracted from the ground at relatively high temperatures, could be used to generate electricity. Additionally, the water, if treated, could be reused for agriculture, municipal and industrial purposes.

#### The Case Study

Mohtar and McCarl will work with the Texas Water Development Board, municipal utilities, agricultural data sources, counties, organizations, and corporations to collect data and build a database for water, energy, population, industrial growth, and food systems in the San Antonio area. Combining McCarl's resources on economic forecasts and climate change trends and with population growth information, this data will be used to generate the initial analysis protocol for the tradeoffs between the proposed future scenarios. Using Mohtar's existing Water-Energy-Food Nexus online platform at www.wefnexustool.org and existing work in the South Central Texas region, Mohtar and McCarl will develop a more comprehensive tool for scenario development and trade-off analysis.

#### Looking to the Future

In the future, Mohtar and McCarl hope to assemble a team that will apply this research to regions across the world. Considering alternative scenarios of water supply, development in the energy industry, regional growth, and climate change, the larger team will offer case study results and provide data for other WEF hotspot regions in the U.S. and internationally.





### Domestication of Microalgae – From Natural Diversity to Synthetic Biology

r: Dr. Arum Han

Associate Professor, Department of Electrical and Computer Engineering

For thousands of years, the natural diversity of physical characteristics and traits in plant and animal species has allowed humans to selectively isolate desirable features for exploitation. In both plants and animals, extended periods of selection can lead to domestication, where a relatively consistent slate of characteristics is present.

In crops such as corn, the selection of desirable characteristics through genetic evaluations and breeding have led to crops that remain appealing to consumers, yet have high tolerances for a range of environmental conditions. The application of these techniques to a wide variety of plants has led to a transformation of crops and harvests around the world.



Associate Professor Department of Electrical and Computer Engineering



Associate Professor Department of Biochemistry & Biophysics

Research like this, however, is at its infancy for single-celled eukaryotic energy organisms like microalgae. Able to produce more biofuel feedstock per acre than any other photosynthetic organism because of their high oil content, algae-based biofuels can be used for transportation needs and are biodegradable. Additionally algae production facilities can be located in a variety of locations that are not used for food production.

However, microalgae is not currently competitive as a biofuel feed stock, partly because of overall low productivity and difficulty in scaling up production from small lab-scale cultures. Shortterm laboratory experiments with optimal conditions indicate that costcompetitive results are possible, but in real-world applications, this efficiency is not often achieved.

To overcome this, algal strains must be generated that can adapt or be suited for varying light conditions, salinity levels, temperature peaks or averages, and the presence of or lack of a competitive landscape.

Dr. Arum Han, an associate professor in the Department of Electrical and Computer Engineering, together with Dr. Timothy Devarenne, an associate professor in the Department of Biochemistry and Biophysics, is working to develop an algal domestication program – a true paradigm shift in the biofuels area. If this "algal breeding" is successful, it has the potential to make microalgal biofuels cost-competitive as an alternative energy source. He and his multidisciplinary team will capitalize on natural diversity to evolve, or domesticate, single-cell green microalgae – using high-throughput engineering innovations – into domesticated biofuel feedstock producers that are tailored to particular environments.

Unlike previous methods, this research will be accelerated by Han's high-throughput engineering innovations, specifically, custom microfluidic screening devices. These devices, or chips, are similar to miniature plumbing systems that allow for manipulation, control, and characterization of millions of cells individually with single-cell resolution control. The single cells showing the most promising traits can be isolated, manipulated, and analyzed in very short periods of time using such microsystems, greatly reducing overall project durations and costs.

For Han's project, the microfluidic devices will be used for two main purposes: facilitate a genome-to-phenome mapping approach and enable directed evolution-on-a-chip.

# Facilitate a Genome-To-Phenome Mapping Approach

The genome-to-phenome mapping approach involves independently identifying the genomes of individual microalgal strains, then identifying the individual physical characteristics, or phenome, of that same strain. Taking dozens of strains from across the world, each are tested under culture conditions such as light, temperature, salinity, and nutrients. With a high number of options and combinations to test, this can only be reviewed efficiently with high-throughput microfluidics analysis.

Han and his group recently developed a microfluidic photobioreactor array capable of high-throughput analysis of microalgal growth and oil accumulation with the ability to provide 64 different culture conditions on a single chip. For this project, he will design and develop a modified platform, which integrates droplet microfluidics, capable of testing up to 1,000 culture conditions at a time.

Single microalgal colony trapped in microstructures for single-cell resolution growth and oil analysis.







#### **Develop Directed Evolution-On-A-Chip System**

Using the observations and knowledge gained in the genome-tophenome analysis, microfluidic devices will be designed to direct the evolution of strains for specific tolerances or characteristics. The microfluidic devices will allow single cells to be tested under increasing levels of stress from radiation, temperature levels, or salinity levels. Particular strains will be identified, sorted, and then reintroduced into the culture chamber for increasing levels of stress to be applied until desired characteristics are consistently achieved. Through this evolution, tailored strains to address numerous stress scenarios could be created, potentially producing "winter" and "summer" variations, or strains that can grow in brackish water or even salt water. Ideally, a library of strains will be created to suit a wide array of implementations.

The diverse team will represent three universities and one national laboratory. Including an electrical engineer, microalgal molecular biologists, a genomics and phenomics expert, and a microagal biofuels expert, the team brings a broad base of experience and the promise of success in a new area.



### **Demonstration of Computer-Aided Design and Discovery of Materials for Energy Applications**

r: Dr. B.A. Wilhite

Associate Professor, Artie McFerrin Department of Chemical Engineering

For materials scientists, the promise of discovering the next new and transformative material is a dream that only requires matching the right elements together under the right conditions. Such a material could address or solve many issues in energy conversion, energy storage, or a host of other applications. Because there are innumerable combinations of elements and material states that could be used, if scientists and engineers want to efficiently minimize their number of iterations and attempts to create these new materials, computer modeling must be exploited.



To model the characteristics and behaviors of new materials, computer simulations attempt to predict how a material will respond to various stimuli or scenarios. Without sophisticated tools and a high inherent accuracy, these computer models are no better than the intuition of a skilled scientist. Therefore, broad-reaching and crosscutting integrated ab initio (Latin: "from the beginning") computational tools and models must be designed and tested for accuracy.

Dr. B.A. Wilhite, an associate professor in the Artie McFerrin Department of Chemical Engineering, along with Dr. Tahir Cagin, a professor in the Department of Materials Science & Engineering, are working to demonstrate that ab initio materials simulations are capable of providing an understanding of the chemistry,

structure, and properties relationships for electroceramics. Wilhite is conducting chemistry-structure measurements and the in-situ electrochemical characterizations, and Cagin is carrying out the ab initio modeling of the proposed materials system.

Specifically, the pair is investigating if density-functional theory (DFT) simulations can accurately model acceptor-doped electroceramics. DFT simulations can be used to simulate the energy surfaces in molecules and are useful in analyzing the potential of materials for use in energy conversion, energy transport, and in energy storage. Wilhite and Cagin will attempt to understand how chemistry and processing conditions dictate the microstructure and phase composition of the materials, they will scrutinize whether the composition and microstructure of electroceramics control the electrochemical properties of materials in larger quantities, and they will investigate whether surface composition and microstructure, combined with the general electrochemical properties, dictate the surface's effect on chemical reactions (catalytic) activity.



Using that knowledge, Wilhite and Cagin hope to determine whether these new materials can be implemented rapidly and effectively to design and create new electroceramics that will lead to transformational advances in energy technology. Such an advancement, a reliable method of cyber-enabled discovery, will bridge the fields of electrochemistry, materials processing, and catalysis.

Focusing on iron-doped barium zirconates, such as  $Ba_{1-x}Fe_xZr_1$ ,  $_yFe_yO_3$ , as a template and platform for demonstration, the feasibility of designing these materials for energy storage and gas processing will be determined. Potential energy storage applications in this route include the management of cyclic loads and capacities associated with next-generation solar power grids through large-scale reversible storage of electrical energy in chemical form with reversible solid-oxide fuel cells. Gas processing applications include advances in natural gas processing and  $CO_2$  mitigation, as well as other electrolysis applications, including  $CO_2$  sequestration and/or monetization as hydrocarbons.

Expanding this investigation further, the simulations, when coupled with the measurements and characterizations, will be combined with optimization and systems analysis to create a "tripod" of development. In this way, Texas A&M researchers will be able to take new materials from concept, to modeling, to characterization, to optimization, and then to final characterization all within the university, in shorter time-scales and with fewer resources than ever before.





Dr. B.A. Wilhite and doctoral student Haomiao Zhang discuss experimental results





# Mesoscale Interactions in the Air Electrode for Li-Air Batteries

Dr. Partha P. Mukherjee

Assistant Professor, Department of Mechanical Engineering

As we look to reduce our carbon footprint and fossil fuel dependence – particularly in transportation fuels – scientists and engineers are working to identify technologies and solutions to overcome the current barriers to vehicle electrification. The primary challenge to vehicle electrification centers on developing



Dr. Partha P. Mukherjee Assistant Professor Department of Mechanical Engineering



Dr. Sarbajit Banerjee Professor



Professor Department of Biology



**Dr. Hong Liang** Professor Department of Mechanical Engineering

rechargeable batteries that will provide enough energy capacity and power to meet or exceed the standards of current combustion engines. A vehicle's energy capacity refers to its driving range, and consumers generally expect vehicles to travel approximately 300 miles on a fill-up or single charge. The power of a vehicle indicates its ability to accelerate at a rate consistent with current vehicles on the road.

Other challenges to vehicle electrification include safety, weight, durability, environmental impact, and a host of additional considerations.

The majority of rechargeable batteries in transportation currently employ lithium-ion (Li-ion) batteries. While providing sufficient specific power to meet consumer expectations, these vehicles generally have a short driving range.

To understand how Li-ion batteries can provide both suitable power and energy, researchers are looking deeply into many areas to exploit this technology. However, batteries are complex, dynamical systems that include a multitude of processes and interactions that are not currently fully understood.

Dr. Partha Mukherjee, an assistant professor in the Department of Mechanical Engineering, has been investigating the multiscale electrode physics of energy storage within Li-ion batteries – analyzing electrochemicalthermal-mechanical interactions and physicochemical processes in battery electrodes, which he calls "electrodics."

He has been investigating the mesoscale physics resulting from microstructure-transport interactions and the dynamic interplay across spatio-temporal, or time and space scales. These investigations have led him to look at other technologies and implementations that may have higher potential for meeting the demand for specific power and energy capacity.

Lithium-air (Li-Air) batteries are an emerging alternative battery technology that shows promise for a revolution to the status quo in electric drive vehicles, potentially providing ten times the specific energy of Li-ion batteries.

Because of this potential, Mukherjee and his research group are expanding their understanding from Li-ion batteries, coupled with expertise in lithium-sulfur batteries and polymer



Mukherjee and his research group are expanding their understanding from Li-ion batteries, coupled with expertise in lithium-sulfur batteries and polymer electrolyte membrane fuel cells, to Li-Air battery technology.

#### Lithium-Sulfur Batteries



**Lithium-Ion Batteries** 





electrolyte membrane fuel cells, to Li-Air battery technology.

A typical Li-Air battery consists of a lithium metal anode, a porous air cathode, and a nonaqueous or aqueous electrolyte. As the battery is discharged, positive lithium ions are formed by the oxidation of lithium at the negative electrode (anode). The positive ions travel through the electrolyte to the positive electrode (cathode) where they react with oxygen to form Lithium Peroxide (Li<sub>2</sub>O<sub>2</sub>) deposits (for nonaqueous Li-air battery) that eventually become a layer. When the battery is charged, the process is reversed. This process only works well, however, when the Li<sub>2</sub>O<sub>2</sub> layer does not become so pervasive in the battery that it inhibits reactions.

Therefore, it is critical to understand the how and why the  $\text{Li}_2\text{O}_2$  forms a layer, so that the layer can be precisely controlled or managed. The complex microstructure of the cathode plays a key role in determining how the ions and electrons flow, how the  $\text{Li}_2\text{O}_2$  layer is formed, and how the  $\text{Li}_2\text{O}_2$  layer behaves.

Mukherjee and his collaborators have hypothesized that the design of the cathode must factor in the interaction of the



To learn how they might prevent the inhibition of reactions and other undesirable outcomes from the Li<sub>o</sub>O<sub>0</sub> deposits and eventual layering, research will be conducted to fully understand why and how the  $\mathrm{Li}_{9}\mathrm{O}_{9}$  is deposited, so that Mukherjee and his team can then control and direct the formation of the Li<sub>9</sub>O<sub>9</sub> deposits and layer. This will be accomplished through mesoscale modeling of the behavior coupled with considerations for microstructural stochastics - the unpredictable and random formation of deposits.

Following that work, electrochemical experiments and nanoscale characterization will be conducted to make associations between the battery's composition and dynamics and the performance of the electrode.

Through this research, Mukherjee and his team hope to outline the basic mechanisms that lead to the formation and accumulation of Li<sub>9</sub>O<sub>9</sub> and how it affects performance within the battery. This understanding will allow engineers to design microstructures that can limit the blockage of pores and other undesirable behaviors during the discharging and charging process. Eventually, this could lead to the development of highly efficient Li-Air batteries with ample power and energy for the future of transportation.





### Integrated Common-Grid Multiscale Models for Seismic Imaging of Subsurface Fluid Flow

r Dr. Richard Gibson

Francesco Paolo di Gangi/Heep Endowed Professorship and Professor, Department of Geology and Geophysics

For many years, as petroleum engineers, geologists, and geophysicists analyzed oil and gas reservoirs deep below the Earth's surface, their characterizations have often been restricted by technology and computational ability. As a result, simplifications to data collection and processing methods were necessary. In recent years, however, advancements in data acquisition, data processing, and in computational modeling are opening new doors to reveal sophisticated tools that may lead us to new frontiers of our understanding of subsurface fluid flow, geological features, and how they interact.



Department of Geology



Professor and Mobil Chair in Computational Science Department of Mathematic



Dr. Eduardo Gildin Assistant Professor and CJ Craft Faculty Fellow Harold Vance Department of Petroleum Engineering

Seismic wave imaging of deep rock formations and reservoirs is now greatly improved by using tens of thousands of sensors, contributing to large datasets with an unprecedented breadth of information. However, despite the proliferation of such data, the level of detail in processed images, or pictures, of the subsurface is limited by physics: seismic wavelengths are normally approximately 100 meters, and processing of seismic wave reflection data relies on simplifying assumptions and numerical modeling to try to achieve higher resolution of detailed geological features.

In the past, analysis from geophysicists was limited because it relied on computer models using uniform, rectangular grids representing earth structures. These small grid cells are approximately 10 to 20 meter cubes in size and are much larger than important geological structures controlling fluid flow. These approaches are used both because of limits in computer power and because the seismic models are based on data received from sensors that are sending waves from the surface of the Earth, down to the reservoir and back up.

The analysis of fluid flow in those same reservoirs, conversely, only needs to consider the reservoir structure and is able to use discretatizations that are often smaller than one meter. The simulations of fluid flow use irregular grids that often have cells that are very thin and perpendicular to geologic layering. This provides a fine scale and highly detailed, yet non-uniform, grid that is well suited to simulating movement of oil or other fluids in the reservoir.



Three-dimensional model of fluid flow in a reservoir using use discretatizations that are smaller than one meter.

Attempting to combine the seismic wave data with the flow data into a single reservoir "map" will present large challenges. Scientists know that the geometry and variations in rock and fluid properties on the fluid flow, or fine scale grid, affect seismic wave propagation as well, and these effects should be included on the coarser scale grid. Unfortunately, there is currently no reliable method to combine these two grids with high accuracy.

Dr. Richard Gibson, the Francesco Paolo di Gangi/Heep Endowed Professor and professor in the Department of Geology and Geophysics, is leading a project to combine these two grids and create a simulator that is built on a common computational grid. This simulator will be a key component of an inversion scheme, a tool that will combine fluid and seismic wave data to characterize a reservoir, providing analysis of porosity and permeability in the subsurface and identifying the distributions of fluid types within the formation.

Unlike analyses of the past, Gibson's approach does not rely on arbitrary analytic solutions that make assumptions or oversimplify subsurface geophysical characteristics and fluid distributions. He will develop integrated multiscale computer modeling techniques to bring together the data for seismic wave propagations and fluid flow analysis. Specifically, Gibson will develop and utilize innovative model reduction schemes, a way to make approximations in the data without making unfounded assumptions.

Beginning with a local model reduction, he will focus on a small area in each coarse grid, called a snapshot space. In this snapshot space, Gibson will identify key characteristics through a technique called local spectral decomposition. Using these key characteristics, he will construct multiscale basis functions, or descriptions of the dominant features of the snapshot area. Multiple basis functions are then coupled through a formulation, and the number of basis functions in each grid is selected adaptively based on estimates within the model reduction. The





combination of the multiscale basis functions yields a common computational grid that will support simulation

This approach could address many problems that are found in the development of energy resources and in the mitigation of associated environmental risks. A reliable means of remotely detecting and quantifying changes to fluids or gases, as well as the pressures within rock formations, could provide critical insights into a reservoir's capacity, aid in decision-making about advanced recovery methods, or even advise future well placements. Seismic imaging is the most important technology for measuring the structure and properties of hydrocarbon reservoir formations between well locations, and time-lapse seismic methods that acquire data repeatedly over time periods of months or years will allow the mapping of fluid movements.

This flow map could present opportunities for measuring the impact of recovery or storage methods well beyond the casing and beyond the reservoir. Extending beyond hydrocarbons, seismic waves can be very sensitive to  $CO_2$ , and potential exists for time-lapse seismic methods to be employed in the monitoring of  $CO_2$  sequestration projects.



# Zephyrgy, A Novel Wind Turbine

**Dr. Othon Rediniotis** Professor, Department of Aerospace Engineering



Dr. Othon Rediniotis Professor Department of Aerospace Engineering



Associate Professor Department of Engineering Technology & Industrial Distribution

As a gentle breeze blows through the trees in your neighborhood, you might not think that this light air movement could power your home. Power generation from wind is often associated with faster wind speeds and large turbines. However, new advances in technology are changing the way wind power is being harnessed, and zephyrs, or light winds, may soon power homes across the country.

The solar power industry has seen significant growth over the last 15 years, particularly in the use of wind turbines for power generation. Many locations across the United States now rely more on wind energy than ever before. However, most of the generation is limited to large wind farms with hundreds of turbines, requiring huge capital investments. Additionally, conventional small-scale

wind turbines do not generally match the efficiency of larger turbines, and small-scale turbines need stronger winds to initiate rotation.

Nevertheless, a demand still exists for small wind turbines that can serve the residential and commercial markets in a cost effective way. Dr. Othon Rediniotis, a professor in the Department of Aerospace Engineering, and Dr. Jorge L. Alvarado, an associate professor in the Department of Engineering Technology & Industrial Distribution, are addressing these challenges with a new small wind turbine called Zephyrgy.

Rediniotis and Alvarado's design is based on standard turbomachinery principles. Zephyrgy is not standard in its design, however. Consisting of a series of up to four rotating rings around a single shaft, the rings contain the blades that spin each stage around the shaft as the air flows through the turbine.

In a conventional wind turbine, the majority of the power produced comes from the outer section of the blades. The Zephyrgy turbine capitalizes on this opportunity by distributing the blades along the widest part of each stage. Each of the rings, or rotor stages, work independently and decrease in size along the shaft, "funneling" the airflow through the turbine and potentially accelerating the airflow to downstream stages under optimum conditions. Because each stage operates independently, each stage can therefore rotate at different air speeds or wind velocities. In this way, even a small gust of wind would activate the smallest of the stages when a conventional turbine would not even rotate.

Zephyrgy improves the efficiency of small turbines and their starting performance by exploiting the wind to its maximum potential with each of the stages. Additionally, the components of the turbines are inexpensive materials that require minimal processing or machining. Ideally, this will lead to a product that is affordable and efficient.



#### Zephyrgy Inner Ring

In this illustration, the magnets rotate with the stage. Electrical coils are mounted on the turbine shaft, which is stationary.

When the stage rotates, the magnets rotate around the coil and produce electricity.

Some components are not illustrated. Not to scale.



# Zephyrgy Wind Turbine

The Zephyrgy Wind Turbine consists of rings, or rotor stages, working independently and decreasing in size along the shaft, "funneling" the airflow through the turbine.





# Exploring the effect of Oil Swelling due to Nanochannel Confinement of $CO_2$ for Enhanced Oil Recovery in Unconventional Reservoirs (Shale)

r: Dr. Hadi Nasrabadi

Assistant Professor and Douglas Von Gonten Faculty Fellow, Harold Vance Department of Petroleum Engineering

In recent years, advances in technology and techniques have opened new doors to the recovery of oil and gas from shale formations around the world. The total worldwide available shale oil resources may be equivalent of more than 5 trillion barrels of oil, and the United States is estimated to have more than 3.7 trillion barrels under its lands and controlled waters. Recovering these "unconventional resources" would greatly expand the world's potential reserves, but recent analysis indicates only 3-10% of this oil is currently economically recoverable.

A small improvement in productivity and recovery could provide access to billions of barrels of recoverable oil.

 $\mathrm{CO}_{2}$  injection has been used to improve oil recovery in conventional reservoirs for the last four decades. The injection of this gas into conventional reservoirs has been proven to aid in oil extraction through three primary mechanisms: beneficial oil swelling, reduction of oil viscosity, and reduction of residual oil saturation.

Injecting  $CO_2$  in "unconventional" shale oil reservoirs is a relatively new concept and the underlying physical mechanisms are still unknown. Several recent studies suggest  $CO_2$  injection





could be a viable method to improve recovery for shale oil reservoirs.

However, the majority of these studies are based on assumptions rooted in experience with conventional reservoirs. Datasets and observations from these reservoirs can be helpful, but computer models and our understanding of CO<sub>3</sub>-oil interactions rely on the behaviors and relationships between the reservoir's contents and the injection fluids and gases at much larger scales than the pores of shale reservoirs. In reality, these assumptions may not be valid, as we cannot conclude that CO<sub>9</sub> and oil interact with each other in the same way in a four nanometer-wide crack as they do in a four micrometer-wide crack.

Dr. Hadi Nasrabadi, an assistant professor and the Douglas Von Gonten Faculty Fellow in the Harold Vance

Department of Petroleum Engineering, along with Dr. Debjyoti Banerjee, an associate professor and the Leland T. Jordan Career Development Professor in the Department of Mechanical Engineering, will perform theoretical and experimental studies to evaluate the confinement effects – the impact that smaller



spaces have on the properties of substances – that shale reservoirs may present to change our understanding of  $CO_2$ -oil interactions. Specifically, the pair will analyze how a confined space affects the solubility of  $CO_2$  in oil,  $CO_2$ 's effectiveness in impacting oil swelling, the viscosity reduction of oil as  $CO_2$  dissolves, and the overall miscibility of  $CO_2$  and oil.

Shale oil reservoirs contain micropores and nanopores with diameters less than two nanometers and some larger pores (mesopores) with diameters from two to 50 nanometers wide. In smaller pores with diameters only a few molecules wide, the surface molecules of the shale may significantly influence the fluid molecules in the pore space. This strong surface-fluid interaction and its competition with fluid-fluid interaction could lead to heterogeneous distribution of fluid molecules throughout the pore space.





Using molecular simulation, Nasrabadi will evaluate the surfacefluid effect on key mechanisms for improved  $CO_2$  recovery in shale oil reservoirs. After the simulation, Nasrabadi and Banerjee will compare the simulations with experimental measurements using a microfluidic and nanofluidic device.

Modeling the  $CO_2$  as it dissolves into the oil under various conditions – particularly the confined space – will allow Nasrabadi to calculate the nanoscale confinement effects on oil swelling and viscosity reduction and how the varying conditions affect the interactions. Additionally, the modeling will permit the calculation of the change in minimum miscibility pressure, which is the pressure at which the interfacial tension between the injected fluid and oil vanishes, or the point at which the oil and  $CO_2$  become a heterogeneous solution. To conduct the experimental measurements, Nasrabadi and Banerjee will construct an adjustable microfluidic and nanofluidic device capable of introducing the  $CO_2$  and oil to a glass microchamber with microchannels and nanochannels. Observations will be carried out through a microscope connected to a high-speed camera. Temperature and pressure modifications to the glass microchamber will be controlled, and will allow the pair to find the minimum miscibility pressure.

The overall objective of the project is an increased understanding of the impact of  $CO_2$  injections as a method of enhanced oil recovery in shale reservoirs. This knowledge has the potential to provide a framework for developing optimum procedures for recovery, and could lead to significant improvements in recovery of resources currently out of our reach.



# **Development of Synergetic/Mobile Multi-source Multi-purpose Ocean Renewable Energy Station**

Dr. Moo Hyun Kim
Professor, Zachry Department of Civil Engineering

As scientists and engineers look to reduce CO2 emissions and the overall environmental impact of energy generation and production, new clean energy resources and new ways of using clean energy resources will play a larger role in the world's energy portfolio.

One promising option that could provide additional clean and renewable power – without waste disposal issues – is the exploitation of the natural phenomena of the ocean, such as waves, wind, currents. Offshore winds are often much stronger and steadier than winds on the land. Floating offshore wind



Professor Zachry Department of Civil Engineering



Dr. Kuang An Chang Professor Zachry Department of Civil Engineering



Dr. James Kaihatu Associate Professor



Dr. Jun Kameoka Associate Professor Department of Electrical & Computer Engineering

turbines (FOWT) are now being deployed at water depths greater than 50 meters.

The ocean's hydrokinetic energy potential through waves and currents presents opportunities around the world to provide power to remote locations, or even to cities through large-scale "farm" implementations. Existing ocean energy conversion systems, however, are far less cost efficient than traditional fossil fuelbased power plants.

Renewable energy sources generally provide power at higher costs than fossil fuel-based power generation plants for many reasons, but several issues play larger roles: consistency of supply, volume of supply, and proximity of supply to consumption sources. With advancements in technology and new paradigms in design, these problems could be reduced.

Advancements could come through the integration of several types of renewable ocean energy sources into one single ocean energy station. Additionally, if this synergetic and multi-source station were to be made mobile, it could meet specific demand as it is requested, or it could be used by the U.S. armed forces to provide energy for a foreign remote location or a mobile offshore military base.

#### A Synergistic Option

Focusing on the synergy between wind and wave energy available in an



Ocean waves and currents present a powerful and consistent opportunity for energy generation.

offshore ocean energy station, Dr. Moo-Hyun Kim, a professor in the Zachry Department of Civil Engineering, is working on a new project with Dr. Kuang-An Chang, a professor in the Zachry Department of Civil Engineering, Dr. James Kaihatu, an associate professor in the Zachry Department of Civil Engineering, and Dr. Jun Kameoka, an associate professor in the Department of Electrical & Computer Engineering.

The project will capitalize on Texas A&M's existing wind and wave energy research facilities, which include the Offshore Technology Research Center (OTRC) and the Haynes Coastal Engineering Laboratory's three-dimensional multidirectional wave tanks. The Ocean Engineering Program at Texas A&M University has been involved in the design and testing of offshore oil platforms for more than four decades. Faculty members have strong experience in modeling of the dynamics and stability of floating structures, mooring and anchor systems in harsh marine environments. In addition, Kim has developed the most advanced FOWT and wave energy converter (WEC) computerbased simulation programs in the world.

Combining the broad knowledge and experience within the team, Kim will lead the development of a synergistic and mobile FOWT platform with an innovative WEC system.



The WEC will incorporate a smart material that will actively respond to changes in wave height or frequency. As the waves fluctuate, the smart material – using computer control – will respond differently and allow for more consistent power production, even with calmer seas.

Kim will be responsible for modeling the interactions between the waves, the platform, turbine(s), mooring, and the anchoring for the global performance simulation. Chang will conduct small-scale laboratory model tests at the Ocean Engineering Wave Tank, a glass walled 2D wave tank that is 115 feet long, three feet wide and four feet deep. Kameoka will be responsible for developing and fabricating the simplified smart material of the WEC, and Kaihatu will be responsible for wave and wind characterization, modeling, and forecasting.

#### **Broader Applications in the Future**

In the future, this research could be expanded for other purposes, further broadening the spectrum of future applications.

Adding ocean current energy collection or solar energy collection could provide additional generation options for the platform. A hydrogen factory could also be incorporated, potentially useful for future hydrogen fuel cell cars, and the hydrogen could be drawn from the ocean water.

Coupling a platform with a land-based desalination plant could provide another strong partnership, where wave energy can provide the needed continuous pumping action to send the highly pressured water flow to the land for processing.

The platform could also be used as a captured CO2 disposal station, allowing for the injection of CO2 into the porous sand layer beneath the seafloor. Finally, an oceanographic measuring station could be added, providing space for wind, wave, current, salinity, temperature, and other observations.

A multi-source station could provide a near-constant supply of electricity, greatly enhancing the commercial value of the entire station. During a period of very low wind, wind turbines might not be able to generate enough electricity to meet demand, but other sources on the station – such as wave, current, or solar – could compensate.

In the future, these clean energy resources present new unique and mutually beneficial ways creating and using clean power – through the natural phenomena of the ocean.









# Texas A&M Research

With more than \$820 million in research expenditures generated by Texas A&M faculty-researchers, the university ranks in the Top 20 of universities nationwide in total research expenditures.

Researchers and graduate students are involved in projects on every continent in the world, with more than 600 initiatives underway in more than 80 countries.

Texas A&M University holds membership in the prestigious Association of American Universities, one of only 62 institutions with this distinction.

The university was named second in the nation by The Wall Street Journal among all universities, public and private, in a survey of top U.S. corporations, non-profits and government agencies, based on graduates that recruiters prefer to hire.

Texas A&M has an endowment valued at more than \$5 billion, which ranks fourth among U.S. public universities and 10th overall.

The campus' 400-acre Research Park includes 10 diversified facilities and more than 500,000 square feet of space for innovative companies and organizations focused on transferring new technologies into the marketplace.

Texas A&M has a history of more than 100 years of research and development activities in the field of energy.



302 J.K. Williams Administration Building | 3372 TAMU College Station, TX 77843-3372 979.458.1644 | energy.tamu.edu