# Welcome to the Center for Carbon Management in Energy's

# Research

## Day 2020

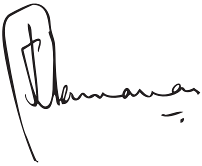
**Welcome to Research Day 2020.**

We are excited to share with you some of the fundamental, curiosity-driven research that is underway the University of Houston. Our undergraduate, graduate and postdoctoral fellow programs are full of bright individuals who are bringing new thought and insight to solve the challenges our industries face.

At UH, research is different. The entrepreneurial spirit throughout our campus has fostered a real drive toward finding commercially-viable solutions and technologies – a developing ecosystem that supports research from ideas to inventions. Part of these activities involve our long-standing partnerships with industries throughout our region. With more than $450 billion in GDP annually, Houston will continue to grow with strong academic-industry/corporate partnerships that value the role of fundamental research in solving the challenges they face.

Let us introduce you to the most important output at the University of Houston – our students. This booklet is full of student and faculty research projects across a multitude of disciplines. These students are mentored by UH faculty scholars, who helped drive the University into high-research activity to better serve our students, our region and our nation. Though this is only a snapshot of our student-research activity, you will get a glimpse of the diversity of our research and the talent our University is supporting as part of our academic mission.

Thank you for your partnership and support. We look forward to connecting with you more in the future to help to move Houston forward.



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# CHEMICAL & BIOMOLECULAR ENGINEERING

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# CHEMISTRY

UNIVERSITY of HOUSTON

# Enhanced Catalytic Oxidation of Methane by Feed Modulation on Pt/Pd/Spinel Monoliths

Methane emissions are problematic in the production of in shale liquid and the use of natural gas as a transportation fuel. In this project a new class of oxidation catalysts are in development to that have a lower Platinum Group Metal (PGM) content.

## Abstract


With increasingly stringent tailpipe emissions regulations from vehicles powered by internal combustion engines, and growing concerns over the use of fossil fuel, Compressed Natural Gas (CNG) vehicles have gained interest [1]. Advantages of CNG vehicles include the use of inexpensive domestic fuel and less $CO_2$ emissions than gasoline and diesel vehicles. The challenge for emission control of CNG vehicles is to simultaneously convert hydrocarbons, CO, and NO into water, $CO_2$ and $N_2$. However, conventional platinum group metal (PGM) based three-way catalysts are ineffective in methane emission control [2]. Four way catalysts (FWC) that can also convert methane need to be developed.

In this study, a novel dual layer (PGM+spinel) monolith FWC (30 PGM g/ft3 monolith, 19:1 ratio of Pt:Pd) developed by CDTi, Inc. is evaluated for methane and NOx conversions performance. $Mn_{0.5}Fe_{2.5}O_4$ spinel was used as the oxygen storage material (OSM). Light-off curves show that the combination of lean/rich feed modulation and the addition of spinel enhances methane and NO conversions. Further experiments studied catalyst design and operating optimization. Parametric studies explored the effects of the oscillation amplitude, average lambda, and oscillation frequency on catalyst performance. Experimenting with intermediate layers showed that the spinel's affects were unaffected by distance to the PGM-layer. Finally, light-off curves with different spinels as the OSM demonstrated that spinel composition has a strong effect on catalytic activity.


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# Enhanced Catalytic Oxidation of Methane by Feed Modulation on Pt/Pd/Spinel Monoliths

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- Joshi, S., Y. Ren, M.P. Harold, and V. Balakotaiah, "Determination of Kinetics and Controlling Regimes for Propylene and Methane Oxidation on Pt/$Al_2O_3$ Monolithic Catalyst Using High Space Velocity Experiments," Ind. Eng. Chem. Res., 51 (22), 7482–7492 (2012).
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# Elimination of Methane and Carbon Dioxide by Catalytic Tri-reforming

The emissions of greenhouse gases carbon dioxide ($CO_2$) and methane ($CH_4$) must be curtailed. In this project the concept of tri-reforming is under investigation as we move towards a carbon-constrained economy. In particular, we are examining the development of a catalytic process that involves the combined reforming of $CH_4$ with $CO_2$ and $H_2O$ in the presence of $O_2$ to syngas (CO, H¬). The focus is on the development of a catalyst and reactor design that minimizes detrimental coke formation while addressing the energy balance and thermodynamic limitations.

## Abstract

Tri-Reforming of Methane is the synergistic combination of Steam and Dry Reforming with the Oxidation of Methane to produce Syngas. A careful balance between these reactions needs to be maintained in order to achieve a desirable yield without deactivating the catalyst. A mixture of reaction conditions and catalyst choices was considered in order to maximize the conversion of Carbon Dioxide and Methane.

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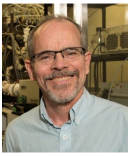

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# Enhancing Methane Conversion over Platinum Group Metals with Tailored Oxygen Storage Materials


## Abstract

In the current energy and environmental scenario, efficient use of energy resources and reduction of greenhouse gases in the atmosphere have garnered a lot of attention. Consequently, researchers are spending substantial efforts toward improved treatment of automotive exhaust, a major source of air pollution. Compressed Natural Gas (CNG) vehicles are becoming prominent as it can potentially lead to lower $CO_2$ emissions due to the higher H:C ratio of methane compared to diesel and gasoline [1]. This technology, however, suffers from unburnt methane emissions, another major potent climate change causal agent. The lack of viable processes converting methane from distributed sources to easily transportable liquids has also led to an increase in flaring, i.e. the total combustion of methane, to lower the environmental impact of enhanced oil recovery. In both these applications efficient methane oxidation/conversion catalysts can greatly incentivize technologies for natural gas/methane capture and use, a major step towards lowering net greenhouse gas emissions.

This study is guided towards a fundamental understanding of methane oxidation process over precious metal (PGM)/metal oxide catalysts. Spinels are a class of mixed metal oxides that can act as excellent oxygen storage materials (OSM). A dual layer (PGM+spinel) monolith (30 PGM g/ft3 monolith, 19:1 ratio of Pt:Pd) developed by CDTi, Inc. has demonstrated higher methane conversion at low temperatures of 300-400 °C than conventional Pd/ceria-zirconia catalyst. A bench reactor system is used to conduct flow experiment using both steady-state and modulated feeds and the effluent concentrations are measured by a Fourier transform infrared (FTIR) spectrometer. These experiments show that the combination of lean/rich feed modulation and the addition of spinel allow for reducing methane conversion temperatures. It has been hypothesized that methane activation follows two principal routes: direct activation over the surface sites of the PGM component, and an indirect route, where the oxide provides oxygen necessary to efficiently activate the C-H bond in methane. Direct methane activation over PGM sites and/or spinel surface metal sites demands high temperatures. The indirect route comprises of PGM sites being the only methane activation centers, with metal oxides simply acting as oxygen reservoir. This allows for easier low temperature methane activation on the PGM sites, located right on the spinel surface. Herein, we present the impact of two OSM materials, $Mn_{0.5}Fe_{2.5}O_4$ spinel and $Ce_{0.3}Zr_{0.7}O_2$ (CZO) on methane activation on PGM over OSM catalysts through pulse-injection method for the dynamic oxygen capacity (DOSC) measurement. Ab initio density functional theory calculations are performed to probe the oxygen vacancy formation and equilibrium oxygen evolution from the spinel oxides due to phase transition under varying oxygen partial pressure. Elucidating the DOSC of these materials can pave the way towards a fundamental mechanistic understanding of methane activation and improved catalyst generation for future.



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# Enhancing Methane Conversion over Platinum Group Metals with Tailored Oxygen Storage Materials

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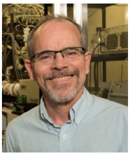


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# Carbonate Assisted Electrochemical Methane Activation on Ni(111) and NiO(100)


## Abstract

Methane, an abundant resource in the U.S., has very strong C-H bonds, which makes its activation energy consuming. Current catalysts used to upgrade methane to higher value products are facing two major issues: (i) high temperatures (up to 900 K) are required, and (ii) the life time of the catalysts is limited due to sintering and coking. We aim to address these challenges and pursue a novel low temperature process, which leverages the use of an electrochemical cell to convert methane to methanol. This solution is particularly interesting for small-scale methane conversion and distributed manufacturing.

The envisioned process uses carbonate anions ($CO_3^{2-}$) that are produced from $CO_2$ and $O_2$ at the cathode and transferred to the anode through an electrolyte. At the anode, carbonate ions serve as activator for methane and transfer a single oxygen atom to selectively oxidize methane to methanol. The fact that carbonate anion reduction leads again to $CO_2$, which readily desorbs into the gas phase, is considered a key advantage of the proposed electrochemical process. The rate of $CO_3^{2-}$ delivery can be controlled by adjusting the cell potential or current density. By simultaneously controlling the concentration of $CH_4$ at the anode, we anticipate that the over-oxidation of methane can be prevented, such that a high yield of methanol can be achieved.
We have performed density functional theory (DFT) calculations on Ni(111) and NiO(100) and explicitly accounted for the effects of applied electric fields. Our results indicate that the interaction between the externally applied electric field and the dipole moment generated between the surface and adsorbates plays the dominant role in altering the binding behavior. Hence, the reaction enthalpy and activation energy of certain elementary steps exhibit a strong dependence on the applied electric field. Although the applied electric field does not lower the activation barrier significantly, the results show the possibility to guide the reaction through a desired direction by altering the applied electric field so that the selectivity of methanol can be increased.

While the development of a viable process remains in its early stages, our results suggest that an electrochemical cell with a tunable electric field offers unique advantages for selectively upgrading methane to value-added products.


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CHBE

# Screening Metal-Oxides for Efficient Oxidative Coupling of Methane

## Abstract

Methane has become an abundant energy resource following the recent developments in the natural gas exploration and extraction technologies. Besides being an energy provider, methane can also serve as a commodity that can be converted to higher alkanes/alkenes. At many natural gas reserve sites, a particular volume of the natural gas may be flared if it is considered uneconomical to obtain. A more lucrative alternative would be converting gaseous methane into liquid higher hydrocarbons as they are more valuable and their transport is more economical than the gaseous methane. Oxidative coupling of methane (OCM) has traditionally been a focal point in methane conversion as it allows for the direct conversion of methane into $C_2$+ products. The biggest drawback of OCM is its limited $C_2$+ yield as the formation of COx byproducts is thermodynamically strongly favored. While there have been several large-scale investigations on experimental OCM data aiming to reveal the most ideal catalyst compositions, the final catalyst suggestions are mostly based on statistical analysis rather than intrinsic structural properties.[1,2,3]

In this study, we have computationally screened several metal-oxides, composed of alkali and/or alkaline earth metals, to identify structural predictors for good OCM performance using DFT level of theory. We have constructed partial potential energy diagrams for crucial OCM reaction steps namely hydrogen abstraction and oxygen vacancy formation and correlated the corresponding energies with fundamental descriptors. Moreover, partial charges on participating oxygens are derived and their correlation with OCM energetics is investigated. Finally, the favorable structural properties that can lead to high OCM performance are suggested.

With the right combination of operation conditions and catalyst choice, some of these suggested catalysts can enable an economically viable and single integrated process for the direct conversion of methane into ethylene, one of the most desired chemical building blocks.

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# Global Commoditization of $CO_2$

# The Case for Dual-Use LNG-$CO_2$ Shipping

## Abstract

Rising anthropogenic $CO_2$ emissions and global temperatures are a technological, social, and political challenge. These necessitate deep decarbonization through carbon management strategies for sustained action. Cost-effective transportation of $CO_2$ from point sources to utilization and storage sites has become a significant bottleneck for effective carbon management. We discuss a new mechanism to achieve international cooperation on carbon management through effective $CO_2$-source and $CO_2$-use or sequestration matching is addressed. The mechanism is founded on utilizing the growth of global LNG trade to transport $CO_2$ over long distances via dual-use vessels that carry $CO_2$ on their return journey following the LNG delivery. A foundational carbon capture, utilization, and storage (CCUS)-based economic model for the utilization of $CO_2$ originating in South Korea and Japan through enhanced oil recovery (EOR)-based sequestration in offshore U.S.is explored. The model sets forth the objectives, scale, costs, and implications for the international trade and commoditization of $CO_2$, as against its current status of a waste product. Further, we will discuss policy considerations which can accelerate the deployment of this model, and the global commoditization of $CO_2$ via dual-use shipping thereof.

## Related Publications


- Datta A and Krishnamoorti R (2019) Opportunities for a Low Carbon Transition-Deploying Carbon Capture, Utilization, and Storage in Northeast India. Front. Energy Res. 7:12. doi: 10.3389/fenrg.2019.00012
- Datta A, De Leon R and Krishnamoorti R, Advancing Carbon Management through the Global Commoditization of $CO_2$ – The case for Dual-use LNG-$CO_2$ Shipping, in review


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# Affordable Distributed Air Capture - Policy Pathways

## Integration with Renewable Wind Energy in W. Texas

## Abstract

Direct Air Capture (DAC) is being mainstreamed as a solution for climate change mitigation, however, uncertainties remain around the long-term costs, energy consumption, and land requirement for at-scale capture. Meanwhile, Texas leads the nation in wind energy generation and has an independent electricity grid. During wind energy overgeneration at night, when supply is significantly larger than demand, the excess electricity is sold at negative prices in the wholesale market. This provides an excellent opportunity to utilize this overgeneration to move high volumes of air through DAC units to enable low-cost DAC. This will alleviate the high cost and energy consumption challenges, allow for the rapid deployment of modular and process intensified DAC units co-located with wind farms to minimize transmission costs, and stabilize the grid. However, significant economy-wide policy support would be required before at-scale deployment of DAC integrated with wind can be realized. We discuss some recent policy and regulatory shifts that are indicative of emerging opportunities of transforming DAC from a cost-center to a profit-center, along with recommended policy pathways that could accelerate the pace of this transition.

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# Techno-Economic Modeling of Dual-Use LNG-$CO_2$ Shipping

## Abstract

Source to sink matching is a critical determinant for the feasibility of Carbon Capture, Utilization, and Sequestration (CCUS) projects as transportation costs scale up with distance. Typically, sources of $CO_2$ like chemical and power plants are not in close proximity to potential use and storage (sinks), thereby rendering CCUS projects infeasible. The use of pipelines to transport $CO_2$ has added excessive capital costs and the threat of sunk capital costs to existing projects. Utilizing the explosive growth of the LNG/LPG shipping industry can substantially lower the costs and de-risk transportation of $CO_2$ for CCUS. In this scheme, importers of natural gas capture $CO_2$ and transport it via specially designed dual-purpose vessels to exporters that have aging fields offshore or near to shore for utilization through enhance oil recovery. In this work, we analyze the techno-economic feasibility of this proposition to present the incentives that dual-purpose ship transport can provide- transportation over long distances at a fraction of prevalent costs, elimination of operating costs for an empty vessel on its return journey, the flexibility to route $CO_2$ where it's needed, and the economic benefit of sequestration.

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# Techno-Economic Modeling of Coupled Direct Air Capture of $CO_2$ and Renewable Wind Energy

## Abstract

Carbon capture technologies that capture $CO_2$ from point sources such as power plants, refineries, and chemical plants or distributed and typically low concentration sources like the atmosphere are being advanced as part of a comprehensive carbon management system. Fundamentally, there are three pathways to capture point source generated $CO_2$. They depend on when and how the $CO_2$ is captured in the combustion process: pre-combustion, post-combustion, and oxy-fuel combustion carbon capture. These processes have been scaled up to minimize the energy required for releasing the $CO_2$ and for operations including pipeline compression of $CO_2$. Such point source capture technologies have demonstrated improvements in energy efficiency through the integration of processes and more recently by application of intensification methods. On the other hand, direct air capture (DAC) methods involve low concentration streams, are intrinsically smaller scale, and are distributed. DAC proves economical when adopting passive technologies to capture $CO_2$. We provide a techno-economic analysis of existing DAC technologies and life cycle analysis to understand the efficacy of these methods to reduce the global carbon footprint. We will also discuss the technical opportunities to modularize and intensify such distributed capture technologies to address energy consumption, high capex costs, and integration of renewable energy sources to provide an alternate pathway for rapid penetration of carbon capture technologies.

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# Enabling Rapid Temperature Swing $CO_2$ Adsorption Through Materials Process & Design

## Abstract

Coal-fired power plants are major point sources of $CO_2$, the addressing of which will require the development of separations options that are a step change from traditional thermally driven technologies. Adsorption-based processes have been proposed as low-cost alternatives to absorption-based ones traditionally used for $CO_2$ capture from power plant flue gas. The achievement of high $CO_2$ purities and recoveries, however, is predicated on rapidly cycling between adsorption and desorption cycles- the execution of which requires adsorbent materials that are endowed with improved adsorption kinetics. This work describes the design of high working capacity supported amine adsorbents, and its integration into a hollow fiber-based process that may create the opportunity for large-scale deployment of Rapid Temperature Swing Adsorption (RTSA) technology for $CO_2$ capture from coal fired power plants.

## Related Publications


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• Li, W., Bollini, P., Didas, S., Choi, S., Drese, J., Jones, C. W., Structural Changes of Silica Mesocellular Foam Supported Amine-functionalized CO2 Adsorbents Upon Exposure to Steam, ACS Appl. Mater. Interfaces, 2 (2010) 3363-3372.

# Autothermal Operation of Catalytic Oxidative Coupling of Methane in Packed-Bed Reactors

## Abstract

Oxidative coupling of methane (OCM) is an attractive route for the direct conversion of methane into value added chemicals. The highly exothermic feature of OCM system leads to complex ignition-extinction behavior that depends on both operating conditions and design parameters. Experimentally observed hysteresis behavior in lab-scale reactors motivated the investigation of the feasibility of autothermal operation for OCM. In steady-state autothermal operation, there is no heat addition to the reactor and there is no intentional heat removal by cooling through reactor walls. The existence of multiple steady-states, and in particular an ignited high temperature (conversion) state is essential for autothermal operation with low feed temperatures or space times. High temperature ignited steady-state can be attained either by reactor scale back-mixing of heat or by interphase gradients leading to particle level ignition. The present work examines the impact of operating variables (space time, methane to oxygen ratio and feed temperature), inter and intra-phase gradients and bed level heat and mass dispersion on the ignition-extinction behavior and C2 product selectivity in catalytic OCM reactors. The scale-up of the process for producing ethylene directly from methane at higher operating pressure is also analyzed.

## Related Publications


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# Biological, Anaerobic Activation of Short-Chain Alkalines in *E. coli*

## Abstract

We are harnessing components of a metabolic pathway found in *Azoarcus* sp. HxN1 and *Desulfosarcina* sp. Bus5 to anaerobically activate sub-terminal C-H bonds of short-chain alkanes via fumarate addition. The resulting alkylsuccinate products can be subsequently metabolized into biofuels or other, higher value chemicals. Using *E. coli* as a host microorganism that is readily genetically modified, we are optimizing conditions for the functional expression of activating enzymes (AEs). These iron-sulfur cluster (ISC)-containing proteins are required to generate the catalytic glycyl radical in partner alkylsuccinate synthases (AlkSyns). Several candidate genes have been cloned and expressed to produce AEs and AlkSyns, for various alkane substrates. Identification of the anticipated alkylsuccinate products required organic synthesis of these compounds, for use as authentic standards in LC-MS analysis. Techniques developed, optimization of biological synthesis conditions, and progress toward improving production will be described.

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# Controlling Silicon and Aluminum Zoning in ZSM-5 for Improved Performance in the Methanol-to-Hydrocarbons Reaction

## Publications


- Ghosh, R., Le, T.T., Terlier, T., Rimer, J.D., Harold, M., Wang, D., Enhanced Selective Oxidation of Ammonia in a Pt/ $Al_2O_3$@Cu/ZSM-5 Core Shell Catalyst, ACS Catalysis, under review
- Hwang, A.*, Le, T.T.*, Shi, Z., Dai, H., Rimer, J.D., Bhan, A., Effect of diffusional constraints on lifetime and selectivity in methanol-to-olefins catalysis on HSAPO-34, J. Catal., 2019, 369, 122
- Shen, Y., Le, T.T., Fu, D., Schmidt, J.E., Filez, M., Weckhuysen, B.M., Rimer, J.D., Deconvoluting the Competing Effects of Zeolite Framework Topology and Diffusion Path Length on Methanol-to-Hydrocarbon Reactions, ACS Catal., 2018, 8, 12
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# Exposing Polar and High Index Facets

## Publications


- M. D. Susman, S. Chinta, J. D. Rimer, In preparation, 'Synthesis of mixed NiO-MgO oxides exposing high-index facets via the molten salt route'.
- M. D. Susman, H. N. Pham, X. Zhao, D. A. West, S. Chinta, P. Bollini, A. K. Datye, J. D. Rimer, In preparation, 'Synthesis of NiO Crystals Exposing Stable High-Index Facets'.
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CHBE

# Large Crystal Growth of Functional Inorganic Materials

## & Multifunctional Crystal Growth and Characterization

## Abstract

Large single crystals - centimeter size - of functional inorganic materials (optical, semiconductor, battery, energy, etc.) are crucial for advanced technologies, and to fully understand the underlying property. The Halasyamani laboratory has extensive crystal growth facilities - top-seeded solution growth, Bridgman, and floating zone - that enables the growth of a range of single crystals. In addition to the crystal growth, his group has the capability to cut, index, and polish the crystals. The crystal growth and characterization capabilities make the Halasyamani laboratory unique in the US.

## Related Publications


- Yu, H., Young, J., Wu, H., Zhang, W., Rondinelli, J.M., and Halasyamani, P.S., The Next Generation of Nonlinear Optical Material $Rb_3Ba_3Li_2Al_4B_6O_{20}F$ - Synthesis, Characterization, and Crystal Growth, Adv. Opt. Mater., 1700840, 2017.
- Tran, T.T., Koocher, N.Z., Rondinelli, J.M., and Halasyamani, P.S., Be-free B-$Rb_2Al_2B_2O_7$ (B-RABO) as a Possible Deep-Ultraviolet Nonlinear Optical Material Replacement for $KBe_2BO_3F_2$ (KBBF), Angew. Chemie, 56, 2969-2973, 2017.
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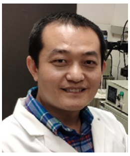

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# COMPUTER SCIENCE

UNIVERSITY of HOUSTON

# High-dimensional Data-driven Energy Optimization for Multi-Modal Transit Agencies

## Abstract

The goal of this project is to develop a high-resolution system-level data capture and analysis framework to revolutionize the operational planning of a regional transportation authority, specifically the Chattanooga Area Regional Transportation Authority (CARTA). There is existing research on improving energy efficiency in transportation networks through analyzing energy consumption data per vehicle type and driving context. However, these studies are based on trip specific estimation and thus cannot be applied to a regional transportation network. Further, a number of these studies are based on simplified model estimation that is used within a simulation framework for analysis and are therefore difficult to validate during actual driving/road conditions that are not captured in the training dataset (which is typically limited in size and features).

The availability of ubiquitous high-speed networking in Chattanooga provides us with a unique opportunity to change this status quo by providing mechanisms to significantly improve the operational efficiency of fleet operations. Specifically, we collect high-resolution datasets containing all information about engine status, vehicle location, fuel usage, etc. in real-time from CARTA's fleet of buses, car sharing, and e-bike sharing vehicles and send them to a central station for analysis. Additionally, we get state of charge data from the electric vehicles, which can then be used to estimate vehicle health using data-driven prognostic algorithms developed by the team. Combined with the traffic congestion information obtained from external sources, such as HERE, this data can help create high-resolution energy consumption predictors, contextualized with features such as vehicle types and events in the city. These predictors can then be used by agencies like CARTA for operational optimization.

Overall, this project will enable the development and evaluation of tools to promote energy efficiency within a mobility-as-a-service transportation model in a mid-sized city. In addition to energy efficiency within each specific mode of operation, such as electric bus and electric car, this project will identify network mobility and energy efficiency associated with movement throughout the continuum of transportation choice present within Chattanooga. Further, the proposed project can complement the DoE national labs effort on vehicle energy consumption model by exploiting new data to investigate impacts of road/driver factors on vehicle energy consumption. In addition, the project can supplement DoE national labs efforts by providing more data on electric bus operations under various driving conditions for model validation.

## Publications

http://aronlaszka.com/publications

# High-dimensional Data-driven Energy Optimization for Multi-Modal Transit Agencies

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# MECHANICAL ENGINEERING

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# INDUSTRIAL ENGINEERING

UNIVERSITY of HOUSTON

# Full Spectrum Solar Thermal Energy Harvesting and Storage by a Molecular and Phase-Change Hybrid Material

## Abstract

Efficient solar thermal energy harvesting and storage are critical steps toward utilizing the abundant solar irradiation that reaches the surface of the earth. Current solar-thermal approaches rely on costly high optical concentration systems, leading to high heat losses by hot bulk materials and surfaces. At the same time, the energy stored in the form of thermal energy has inherently large temporal losses. Herein, we combine the physics of molecular energy and latent heat storage to introduce an integrated harvesting and storage hybrid paradigm for potential 24/7 energy delivery. The hybrid paradigm utilizes heat localization during the day to provide a harvesting efficiency of 73% at small-scale and ~90% at large-scale. Remarkably, at night, the stored energy by the hybrid system is recovered with an efficiency of 80% and higher temperature than that of the day, in contrast to all the state-of-the-art systems. The integrated hybrid concept and the system open a path for simultaneous harvesting and storage of solar-thermal energy for a wide range of applications, including power-generation, desalination, and distillation.

## Publications

- Full spectrum solar thermal energy harvesting and storage by a molecular and phase-change hybrid material, Joule, 3 (12), 3100-3111, 2019.

## Research Team

- Varun Kashyap
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ME

# CFD Analysis of Windcatchers

## Abstract

Windcatchers, or windtowers, are vernacular architectural elements employed in the Middle East, which ``catch'' the oncoming wind and redirect it inside a building for refrigeration and ventilation. Windcatchers are mostly passive and in their operation provide a HVAC system that is extremely energy efficient. But even if windcatchers exist for over three thousand years, there is abundant discrepancy about the key parameters in determining their efficiency. Namely, the design geometry varies across the regions of adoption, and the different roles of humidity, natural convection and the oncoming wind in driving the flow have not been untangled in the present literature. We simulate barebones models of windcatchers using computational fluid dynamics simulations. We have assessed the effects of tower shape and size on the generation of drafts. We also show how the presence of domes helps getting rid of hot, light air. These exploratory simulations have provided a first set of barebones models to test in the wind-tunnel.

## Research Team

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# Permian Flaring of Natural Gas: Opportunities and Challenges

## Abstract

Most natural gas production in the Permian is associated gas – produced along with crude oil. There is not adequate capability to evacuate the gas and ship it to other locations for the use in traditional applications. As such the gas is either vented or flared. The amount of vented or flared gas from the Permian has been growing. This will only increase over time as Permian crude is forecast to increase in the near future.

The objective of the study is to understand the amount of gas produced, vented and flared currently and in the near future, at a more granular level and to utilize the information to develop gathering systems to collect the gas in a central place(s). The study also plans to develop options (viability and economics) to properly utilize the gas – mainly focus on transport via pipelines, use for local power generation, convert the gas to chemicals.

This study is ongoing and this report is a progress to date.

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# PETROLEUM ENGINEERING

UNIVERSITY of HOUSTON

# Carbon Capture & Storage in Depleted Gas Fields Along the Texas Gulf Coast

## Abstract

Easily available information suggests that many depleted gas fields exist along the Texas Gulf Coast and many refinery operations in the area may include processes that could enable relatively cost effective $CO_2$ capture. This research explains advantages of storage in sufficiently large depleted gas fields related to existing well and pipeline infrastructure and the potential that pressure monitoring would be sufficient to guard against leakage. Further, we describe conditions under which 45Q tax credits make such projects profitable.

## Publications

We hope to publish several papers on or related topics to this research.

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PE

# Development of First CCUS Project in Indian Oilfield

## Abstract

This work summarizes the prospect of EOR and carbon sequestration, by injecting anthropogenic $CO_2$ into an Indian mature oil field in Assam. This work include laboratory study, reservoir static modeling, dynamic simulation, pilot design, and techno-economic sensitivity studies. It was confirmed through PVT laboratory studies that $CO_2$ injection can achieve the miscibility under reservoir conditions. Based on the results from $CO_2$ EOR simulation study, we identified a pilot pattern area of ~ 60 acres with one injector and four producers. The $CO_2$ was injected into reservoir at 150 metric ton per day for 5 years and cumulative injection volume is 15.4 BCF. Then the well is switched back to water injection afterward. Around 1 million STB incremental oil recovery was obtained in about 10 years, which corresponds to 11% of original oil in place in the flooded area. The $CO_2$ utilization ratio is approximately 6 MCF/BBL. It is expected that $CO_2$ flooding yields a pre-tax net cash flow of US dollars of 9.4 MM. CO2-EOR and storage in this mature field has a great techno-economic prospect.

The investigation of CCUS opportunity and the substantial advancement in $CO_2$ flood pilot design project have created an excitement in Indian Oil& Gas industry since the CCUS can significantly improve the domestic oil production from mature oilfields, and also reduce the carbon footprint in India. The volume of anthropogenic $CO_2$ injection and storage in the reservoirs presents the great social and economic benefits for CCUS in India.

## Publications

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- S. Balasubramanian, P. Chen, S. Bose, A. Alzahabi and G.C. Thakur, "Recent Advances in Enhanced Oil Recovery Technologies for Unconventional Oil Reservoirs", OTC-28973-MS, paper presented at Offshore Technology Conference held in Houston, TX, April 30-May 3, 2018.

- A. Deka, P. Chen, and G.C. Thakur, "Diagnostic Analysis Approach to Evaluate Waterflood Performance and IOR/EOR Screening in Mature Reservoirs", SPE Trinidad and Tobago Section Energy Resources Conference 2018, June 25-27. 18TTCE-P-395-SPE.

- G. M. Thomas, A. Selveindran, A. Alzahabi, S. Bose, S. Balasubramanian, G. Thakur: "Improving the Recovery of a Mature Permian Basin Oil Field: An Application of Integrated Petroleum Reservoir Management", SPE-191234-MS, SPE Trinidad and Tobago Section Energy Resources Conference 2018, June 25-27.

- Anand, P. Chen, S. Bose, S. Balasubramanian, G.C. Thakur: "Petrophysics-Driven CO2 EOR Scoping Study: A Field Case Demonstration", presentation and publication at the SPWLA 59th Annual Symposium in London, UK on June 2-6, 2018

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- G. C. Thakur: "Advanced technique for screening EOR (Enhanced Oil Recovery) and IOR (Improved Oil Recovery) methodologies for a given petroleum reservoir". US Provisional Patent Application Serial No UHID: 2017-039, May 15, 2017.
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- G. C. Thakur: "The New Conventional", The Way Ahead Magazine, SPE, 2012.
- Permata, P. and Hatzignatiou, D.G.: "Revitalizing Small Offshore Oil Assets – Field Redevelopment Feasibility Study," J. of Pet. Sci. & Eng., 76, 3-4, 155–171 (March 2011); doi:10.1016/j.petrol.2011.01.007. https://doi.org/10.1016/j.petrol.2011.01.007.
- G. C. Thakur: "The Role of Integrated Project Teams Applying Innovative Technologies to Improve Production and Recovery", pages 5-12, Investigations in Geophysics No. 15, Methods and applications in Reservoir Geophysics, 2010.
- Hatzignatiou, D.G. and Lu, Y. "Feasibility Study of $CO_2$ Immiscible Displacement Process In Heavy Oil Reservoirs". PETSOC-94-90 Petroleum Society of Canada, Annual Technical Meeting, Calgary, Alberta, 1994.
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# CCUS in the Grayburg Formation, Permian Basin

## Abstract

The purpose of this study is to optimize the field development plan (FDP) and $CO_2$ injection in the Grayburg formation in the South Cowden field, integrating production history, geoscience, reservoir engineering and completions data with economic analysis. The South Cowden field is a mature producing onshore oilfield located in the Permian Basin, West Texas. The area under study is a sector of a larger field, and is limited to the Grayburg formation, a tight carbonate zone. The field commenced production in the 1940s and was heavily waterflooded since the 1960s.

This work is built on petrophysical studies, waterflooding analysis and simulation modelling. The key challenges in developing this field are the low productivity of the rock, the high water-cuts in existing wells, and the likely high residual oil saturation remaining. Taking into account these various factors, several economic options were developed to optimize recoveries from the sector studied. One option is the recompletion, reperforation and re-fracking of existing strings, which could add 0.05 MBO incremental reserves. Second, the drilling of infill wells and conversion of existing producers into injectors to optimize water flood yielded an additional 0.5 MBO incremental reserves. $CO_2$ flooding was also investigated and simulation work showed that the use of a $CO_2$ – WAG scheme yielded up to 0.62 MBO additional reserves. The capability of storing $CO_2$ in the Grayburg formation in the South Cowden field was also estimated in this study.

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PE

# Experimental Study of Unconsolidated Sand Yielding Behavior for $CO_2$ Injection-Storage Applications

## Abstract

During $CO_2$ injection and storage operations, reservoir rock goes through decreasing (unloading) and increasing (loading) effective stress conditions. Ramifications of this stress hysteresis loop (loading and unloading cycle) on deformation and fluid flow for unconsolidated sand reservoir are not well understood. They affect $CO_2$ injectivity and containment risk; thereby, the injector design and performance. The simplest model assumes the mechanical behavior is the same for both loading and unloading conditions. In this study we tested this assumption experimentally using test samples made with unconsolidated sands (no cementation) and under different stress unloading (magnitude and path) conditions.

We mapped the loading yield surface with a multi-stage triaxial test with yield criterion of point of positive dilatancy. We then studied the yield behavior under two unloading stress paths of Constant Axial stress test (CAT) (reducing mean stress and increasing shear stress) and Constant Shear stress Test (CST) (reducing mean stress and keeping shear stress constant). Results showed the unloading-based yield surface is also stress path and stress magnitude dependent. However, the unloading and loading based yield surfaces are not the same. For the CAT stress path, the unloading yield criterion is the same as the loading yield criterion. While for the CST, the yield criterion is different than the loading yield criteria and this stress path is being investigated further.

Our tests results showed the loading and unloading-based yield surfaces are not the same. This highlights the needs to determine constitutive model of reservoir rock for representative unloading stress paths. They provide essential results for injector design, prediction of injection performance, and development of safe injection operation envelop for applications of CO2 injection-storage projects. We are planning additional tests to study the combined effects of stress magnitude and unloading stress path on the yield surface of unconsolidated sand and its effect on permeability of the unconsolidated sands. The results of this research are intended to update the simulation software and account for stress path and stress magnitude effects while performing simulation for injectors.

## Publications

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• Wong, G.K., Dudley, J.W., Golovin, E., Zhang, H., and Chudnovsky, A. (2017), "Injector Completion Performance under Hydraulic Fracturing and Matrix Flooding Conditions into a Sand Pack," ARMA 17-0705 presented at the 51st US Rock Mechanics/Geomechanics Symposium held in San Francisco, California, USA, 25-28 June, 2017

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• Mao, D., Karanikas, J., Fair, P.S., Prodan, I.D., and Wong, G.K., (2016), "A Different Perspective on the Forchheimer and Ergun Equations," 180920-PA, SPE Journal Paper, 21 (5) – October 2016

# Experimental Study of Unconsolidated Sand Yielding Behavior for $CO_2$ Injection-Storage Applications

## Publications - Continued


- Zhang, H., Chudnovsky, A., Wong, G.K., and Dudley, J.W., (2013), "Statistical Aspects of Microheterogeneous Rock Fracture: Observations and Modeling," Rock Mechanics and Rock Engineering, Vol. 46 (3) - May 1, 2013.
- Jasarevic, H., Chudnovsky, A., Dudley, J.W., and Wong, G.K., (2009), "Observation and Modeling of Brittle Fracture Initiation in a Microheterogeneous Material," International Journal of Fracture (2009), 158 (1): 73-80. (Download 131)


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PE

# A Hierarchical Model for Predicting the Geo-Mechanical Properties of Carbonate Formations


## Abstract

The geomechanical characterization of a carbonate reservoir is required for formation stimulation and hydrocarbon recovery. The pertinent core- or block-scale (large-scale) characterizations are time consuming and expensive, and more importantly, cannot be used for drill cuttings. The present study proposes a two-scale model based on microscale (small-scale) measurements to predict the geomechanical properties of a carbonate formation at the core scale. At the small scale, we develop a physically representative element by accounting for the effective stiffness of a constitutive mineral and of voids. At the large scale, we account for the volume fraction of each mineral, the porosity, and the pore structure of the void space. The elastic deformation of a large-scale model is simulated using a finite element method (FEM), whose results are tested against independent lab measurements. The proposed two-scale model has applications for geomechanical characterization of a formation at the core scale from drill cuttings.



Sponsored by: Qatar Foundation


## Publications


- Esatyana, Erica., Li, W., and Sakhaee-Pour A., A Hierarchical Model for Predicting the Anisotropic Elastic Moduli of Shale Formations. (submitted).
- Sakhaee-Pour, A., and Li, W. (2019). Two-scale geomechanics of shale. SPE Reservoir Evaluation & Engineering, 22(01), 161-172.
- Li, W., and Sakhaee-Pour, A. (2018). Two-scale geomechanics of carbonates. Rock Mechanics and Rock Engineering, 51(12), 3667-3679.


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PE

# Candidate Selection for $CO_2$ Storage Insights from Pore-Scale Modelling


## Abstract

For decades, $CO_2$ has been injected int subsurface formations for various purposes, mostly to enhance oil recovery from such formations. While the energy industry perfected $CO_2$ enhanced oil recovery technology, the rise of global warming and carbon management necessitates a similar but technically unique scenario for Energy companies – reinject $CO_2$ into formations, not for enhancing oil recovery, but for permanent storage. This study presents research findings on the pore scale behaviour of $CO_2$ when injected into such formations. Preliminary analysis involves characterization studies for digital equivalents of case study Bentheimer sandstone sample using ImageJ. Using the D3Q15 Lattice Boltzmann algorithm, flow is studied in this formation primarily to assess its capability for capillary trapping, a major mechanism of $CO_2$ retention. The sample is flooded up to 1.5 pore volume. Saturation distribution at different stages are presented. It is shown that assessing a storage reservoir requires a tradeoff between the permeability needed for $CO_2$ flow, and sufficient tightness for $CO_2$ retention.


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PE

# PHYSICS

# PUBLIC POLICY

UNIVERSITY of HOUSTON

# Carbon Dioxide Recycling and Carbon Free Fuel Production Using Sunlight

## Abstract

The new millennium has been witnessing a variety of historically unprecedented environmental problems including a dramatic increase in the atmospheric carbon dioxide level and average global temperature, a decrease in the arctic ice coverage and an increase in the sea level. Recent studies link these changes with the emissions due to human activities. Carbon dioxide recycling by converting it back to fuels and production of carbon free fuels such as hydrogen from water using renewable sources are potential strategies. Among the solar fuel generation technologies emerged in recent years, photocatalytic and photoelectrochemical routes are highly promising. The photocatalytic properties of semiconducting materials are utilized in these technologies for the conversion of energy in the ultraviolet to near infrared region of the solar spectrum to chemical energy. While many photocatalysts used in these processes lack the ability to either absorb sunlight in a broad energy region or convert the absorbed energy efficiently to fuels, other materials suffer from stability problems. We recently demonstrated that these problems could be addressed by combining 0, 1 and 2 dimensional (0, 1, 2D) architectures of photocatalysts. A unique nano-heterostructure formed by joining titania nanotubes (1D) with a few new 2D and 0D materials exhibited broad spectrum light absorption and utilization for solar hydrogen generation. This presentation will give the details of our recent efforts to develop such nano-heterostructures for efficient solar fuel generation.

## Publications

- S. Radhakrishnan et al. Fluorinated boron nitride quantum Dots: A new 0D material for energy conversion and detection of cellular metabolism, Particle & Particle Systems Characterization, 36, 1800346 (2019).
- A. P. Balan et al. Exfoliation of a non-van der Waals material from iron ore hematite, Nature Nanotechnology, 13, 602-609 (2018).
- A. P. Balan et al. A non-van der Waals 2D Material from natural titanium mineral ore Ilmenite, Chemistry of Materials, 30, 5923-5931(2018).
- O. K. Varghese, Sunlight for fuel generation via carbon dioxide recycling, Nanomaterials and Energy, 4, 244-255 (2013).
- O. K. Varghese et al. High-rate solar photocatalytic conversion of CO2 and water vapor to hydrocarbon fuels, Nano Letters 9, 731-737 (2009).

## Research Team

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PHYS

# Non-Precious Electrocatalysts for High-Performance Alkaline Seawater Electrolysis

## Publications

- Non-noble metal-nitride based electrocatalysts for high-performance alkaline seawater electrolysis

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# The Oil & Gas Workforce of the Future

## Abstract

We conducted an online survey of UH students who are likely to consider a future career in the energy industry. The purpose of this survey is to understand how potential employees in the energy industry perceive corporate social responsibility (CSR) and how CSR influences their employment decisions. A total of 608 respondents completed the survey. A majority of respondents say CSR and environmental stewardship plays an important role in their employment decisions in the oil and gas industry. When evaluating hypothetical job offers, the importance of environmental stewardship remains and is very substantial, even after taking into consideration the type of industry and starting salary. Students in technical fields such as petroleum engineering, and students in social science, business and humanities, all view corporate social responsibility as important to their employment decisions.

## Publications

- Ryan Kennedy and Pablo Pinto. 2019. "Insights into the Oil and Gas Workforce of the Future." UH Energy Whitepaper Series: No. 03.2019.

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