HYDROGEN RESEARCH FIRST LOOK A glimmse into the

A glimpse into the latest faculty, graduate, and postdoctoral hydrogen-related research at the University of Houston



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Graduate School
Office of the Provost

ELECTROCHEMICAL CARBON CAPTURE USING AMINES REVIVING ABSORBENT CHEMISTRY OF AMINE TO IMPROVE THE ENERGETICS OF ELECTROCHEMICAL DESORPTION

RESEARCH ABSTRACT

This study investigates the absorbent chemistry of Electrochemically Mediated Amine Regeneration (EMAR) for carbon capture by exploring secondary amines. previously overlooked due to weak metal-amine interactions. It specifically examines how blending secondary amines—MEA, AMP, MDEA—with ethylenediamine (EDA) affects EMAR's efficiency. The EDA+MDEA combination outperformed others, reducing charge transfer resistance by 40% and tripling the electron transfer rate. It also significantly decreased desorption energetics to 37 kl/molCO_2 , a 34%improvement over pure EDA. scale-up of EMAR for point source carbon capture.

FIGURES





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EDA+NDEA

20



ACHIEVING OFFSHORE MICROGRID ENERGY INDEPENDENCE: OPTIMIZED ON-SITE RENEWABLE RESOURCE CAPACITY

RESEARCH ABSTRACT

Offshore oil and gas platforms primarily use fossil fuels for power, contributing to 15% of global energy-related CO2 emissions in 2023. To decarbonize, many O&G companies are shifting towards offshore clean energy microgrids. Adopting these microgrids aim to meet energy needs efficiently and reduce carbon footprint. The Cost Optimization Renewable Sizing (CORS) model optimizes the sizes of renewable resources like solar, wind, tidal, and wave energies, coupled with battery and hydrogen storage systems, considering variability of generated power and costs. Simulations show substantial cost savings and sustainability advantages while ensuring reliability.

FIGURES



Fig. 1. One-line Diagram of clean energy microgrid



Fig. 2. Average power output of (a) TEC (b) WEC (c) OWT (d) FPV



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WATER ELECTROLYSIS FOR EFFICIENT HYDROGEN PRODUCTION

RESEARCH ABSTRACT

The U.S. Department of Energy (DOE) launched the Hydrogen Energy EarthShot aiming to reduce the cost of clean hydrogen to \$1 per kilogram by 2031. However, a recent report from McKinsey revealed that instead of declining, the cost of clean hydrogen increased in 2023, prompting a revised target for green hydrogen of \$2.5-4.0 per kilogram in 2030, well above DOE's initial target [1]. This underscores the urgent need to reduce the cost of green hydrogen production. Among various membrane-based water electrolysis techniques, Anion Exchange Membrane Water Electrolysis (AEMWE) holds phenomenal potential to reduce the levelized cost of hydrogen (LCOH). AEMWE combines the advantages of both the usage of low-cost Platinum Group Metal (PGM)-free catalysts, such as Alkaline Water Electrolysis (AWE), and high-purity hydrogen production at high current densities, such as Proton Exchange Membrane Water Electrolysis (PEMWE). In pursuit of low-cost, efficient, and stable AEMWE, our group has pioneered systematic research on the synthesis of state-of-the-art non-PGM catalysts, pretreatment-enabled seawater electrolysis, development of highly conductive and durable Anion Exchange Membranes (AEMs), and holistic optimization of AEM electrolyzer design. With our comprehensive skills and approaches, we have successfully designed and fabricated AEM electrolyzer stacks, able to operate stably under industrial conditions with record-low voltages.

[1] Hydrogen Council, McKinsey & Company. (2023). Hydrogen Insights December 2023. https://hydrogencouncil. com/wpcontent/uploads/2023/12/Hydrogen-Insights-Dec-2023-Update.pdf



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TECHNOECONOMIC AND LIFE CYCLE ANALYSIS OF HYDROGEN

RESEARCH ABSTRACT

Hydrogen is a promising clean energy carrier crucial for transitioning to a sustainable, carbon-free energy system. Traditional methods like steam methane reforming emit carbon dioxide, contributing to global warming. Our programs will use Technoeconomic (TEA) and Life Cycle Analysis (LCA) to examine green-house gas and other sustainability footprints of hydrogen production and use. These analyses will support industry and policy makers in optimization and decision making for decarbonization of the global economy for energy and chemicals.

FIGURES



Fig 1: Climate impact associated with the production of NG-based hydrogen (Bauer et al., 2022.)



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TRANSIENT KINETIC OPTIMIZATION OF HYDROGEN YIELD DURING METHANE PARTIAL OXIDATION

RESEARCH ABSTRACT

Microkinetic modeling in heterogeneous catalysis has been advancing substantially in its ability to provide results that qualitatively or even semi-quantitatively agree with experimental observations of reaction kinetics. While many kinetic studies are limited to steady-state observations, dynamic reactor operation results in surface coverages and catalytic regimes that can greatly outperform steady-state operation. We use transient microkinetic modeling to examine the potential of using forced dynamic operation through feed modulation to enhance the yield to H2 during partial oxidation of methane over Pt catalyst. In our model, we impose dynamic conditions by cycling the inlet feed composition between lean and rich conditions. The model results are anlyzed with focus on the oxygen surface coverage and how it affects the surface chemistry. To increase the quantitative prediction accuracy of our kinetic model, we use Bayesian Estimation to tune the kinetic parameters where the uncertainty from experiment and theory are considered together to generate a consolidated "good guess" for the fitted parameters. Ultimately, the model will be used to predict dynamic operating strategies that maximize the cycle average yield to H2 from partial oxidation of methane.

FIGURES



Figure 1 (left): Feed mixture containing 2% CH₄ and (b) 0.05% O₂, (c) 0.1% O₂, (d) 0.2% O₂, (e) 0.5% O₂, (f) 1% O₂, with the 2nd phase containing 1% O₂ Figure 2 (right): CSTR outlet pressure profile for 2% CH₄ and (a) 0.05% O₂, (b) 0.1% O₂, (c) 0.2% O₂, (d) 0.5% O₂, (e) 1% O₂ inlet feed composition





Figure 3: Turn over frequency for methane partial oxidation in CSTR containing 2% CH4 and (a) 0.05% O2, (b) 0.2% O2, (c) 0.5% O2, (d) 1% O2 inlet feed composition



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HYDROGEN STORAGE-BASED MICRO WATER ENERGY NEXUS

RESEARCH ABSTRACT

This project proposes the use of hydrogen energy storage (HES) for back-up power during main grid failures for a micro water-energy nexus (MWEN) in coastal communities with the intent of reducing the use of back-up diesel generators, achieving cost and environmental benefits. The project formulates a mixed-integer linear program (MILP) that optimizes operating cost of the MWEN and is used to compare the total cost of a MWEN with only a diesel generator as back-up, and one with both generator and HES. The results show substantial operating cost reductions achieved by enabling the HES as reserve for unforeseen contingencies.

FIGURES



Fig. 1: Back-up diesel gen. use for a) base case, and b) HESS Case, for 20% reserve of second comparison.



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OPTIMAL OPERATION STRATEGIES OF HYDROGEN FACILITIES IN RENEWABLE ENERGY-DOMINATED POWER GRIDS

RESEARCH ABSTRACT

Our research introduced a daily operation model for integrated hydrogen transportation and storage grids, exploring the benefits of hydrogen facilities. We also developed an Annual Scheduling Model (ASM) for integrating Seasonal Hydrogen Storage (SHS), optimizing hydrogen exchange both within and across seasons through energy hubs that include salt caverns, electrolyzers, and fuel cells. Our numerical results validate that these models can reduce costs and mitigate renewable energy curtailments, highlighting the potential of hydrogen facilities to support future grid sustainability.

FIGURES



Fig. Comparison of Total Conventional Energy Generation Across Different Quarters



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UH ENERGY TRANSITION INSTITUTE

RESEARCH ABSTRACT

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- Hydrogen
- Circularity
- Carbon Management

FIGURES





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RESEARCH ABSTRACT

This research proposes an offshore Hydrogen Energy Storage System (HESS) to interface with subsea oil and gas production systems and offshore renewable energy sources (like wind, floating solar, etc.). Such a HESS will provide a stable energy supply for an extended period, reducing the need for carbon-heavy backup systems such as diesel generators, thereby resulting in a much cleaner energy future. The proposed offshore architecture is modeled using a Hydrogen Energy Storage System (HESS) along with offshore renewables (primarily wind energy), subsea loads (such as drives for pumps, compressors, etc.), and a medium voltage DC (MVDC) grid. Each unit of the HESS is constructed using an electrolyzer to produce hydrogen from electricity, a hydrogen tank to store the fuel, and a fuel cell to transform hydrogen back into electrical energy. Each unit has separate converters to step up/down the voltage. These units are further interconnected through a multi-level cascaded bridge architecture to achieve a 6 kV output. The multi-level cascaded bridge architecture ensures the reliable operation of the system by re-balancing the energy storage electrically between the cascaded mode and protecting the system from any misshape that happens in the system. Suppose a fault occurs in one of the fuel cell units. In that case, the cascaded bridge architecture disconnects that unit from the system. It compensates for that unit by recovering the difference voltage from the other units to maintain the 6 kV DC output voltage.

FIGURES





Multi-Level Converter Architecture for Hybrid Storage Systems

Hybrid ESS Architecture for DC Grid/Microgrid



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SUSTAINABLE MICROGRID SYSTEMS USING HYDROGEN AS AN ENERGY CARRIER

FIGURES (CONT'D)



Fault-tolerant Multi-level Converter System



Simulation Results of output voltage of each boost converters (modules)



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SYNTHETIC AND KINETIC STUDY OF COATED WIRES FOR ELECTRIFIED STEAM METHANE REFORMING

RESEARCH ABSTRACT

Replacement of conventional Steam methane Reforming reactors with Electrically/ resistively heated reactors that are compact and modular would allow for decarbonization of H₂ production. Specifically, parallel wire configurations enable uniform current distribution and high thermal efficiencies. The catalytic structure developed must be thermally stable with sufficient activity under joule heating conditions, especially during fast start-up and shut-down procedures. In the current work, we overcome challenges to successfully synthesize FeCrAl-coated wire catalysts by optimizing parameters of catalyst slurry, achieved uniform active metal distribution with coat thickness 8-12 µm. Lifetime and stability of the coated catalyst is analyzed and seen 70% conversion at 600°C. Since, the understanding of kinetics and mechanisms is crucial to optimization and scaling up of electrified reactors, we try to identify key intermediates and explaining inhibition effects using these electrified coated catalysts that mediates overall H₂ yield.

FIGURES



Configurations of Electrified reactor



SEM image of coated catalyst



Stability test during reforming conditions



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INTEGRATION OF HYDROGEN IN TEXAS Power Grid

RESEARCH ABSTRACT

As Texas experiences a surge in hydrogen production demand, operators are facing challenges in reducing energy costs and curtailment. These challenges are caused by a supply-demand mismatch, feeder congestion, and nodal voltage limits. Converting surplus renewable electricity into hydrogen through electrolyzers has been recognized as a potential way to address these issues. In this research, we investigate the effect of the increasing demand for hydrogen on the Texas electricity network. Our numerical simulations show that the introduction of hydrogen demand can utilize renewable power and requires upgradation of ERCOT electricity network.

FIGURES





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ROOM TEMPERATURE SYNTHESIS OF HYDROGEN PERMEATION BARRIER FOR NATURAL GAS INFRASTRUCTURE

RESEARCH ABSTRACT

Carbon steel is the most common of four steel grades in the United States accounting for 90% steel production. This alloy is designed to be used in industrial applications including oil and gas pipelines due to its high strength-to-weight ratio and formability. However, the diffusion of hydrogen into the material leads to damage and degradation due to hydrogen embrittlement. For this reason, designing surface treatment hydrogen barrier coating seems necessary, and we have conducted our research on the benefits of copper coating as an effective hydrogen permeation barrier. To achieve this goal, we have developed room temperature, electroless process (chemical deposition) for high-quality Cu-based hydrogen permeation barrier films on the surface of A36 carbon steel. The hydrogen interaction with this alloy has been characterized using an electrochemical permeation test and the properties of the A36 carbon steel sample with and without coating were analyzed and compared.

FIGURES





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NATIONAL HYDROGEN TRANSPORTATION FUEL SUPPLY

RESEARCH ABSTRACT

Hydrogen (H_2) fuel cell electric vehicles (FCEVs) refuel in less than 5 minutes with water vapor as their only exhaust emission and are more energy efficient than internal combustion engine vehicles (ICEVs). Consequently, they represent potentially attractive alternatives to battery electric vehicles (BEVs) and ICEVs. However, rare access to H_2 refueling limits this choice in the United States (US). This research assesses the viability of switching from liquid fuels to H_2 at all locations in the contiguous US and will provide a methodology for estimating the competitive price of H_2 in US locations.

FIGURES





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SCREENING OXIDE NANOPARTICLES FOR OXYGEN EVOLUTION REACTION USING THE OPEN CATALYST PROJECT

RESEARCH ABSTRACT

The chemical space for candidate oxides in OER is restricted due to highly acidic reaction conditions. We propose nanoscale stabilization as a possible solution to tackle these restrictions. Using machine learning potentials in the OC22 framework, we predicted phase diagrams to identify synthetically accessible oxides at the nanoscale. We then predicted the overpotentials of these oxides to gauge their viability as electrocatalysts for OER.

FIGURES



Figure 1(Left) High throughput screening framework for identifying oxide catalysts for OER. (Center) Overpotential heatmap as a function of reaction energies of oxides. (Right) Nanoparticle phase diagram depicting stabilization of unstable polymorphs over stable polymorphs at the nanoscale.



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PRODUCTION OF H2-RICH SYNGAS FROM RDF: GASIFICATION VS. CO-PYROLYSIS

RESEARCH ABSTRACT

The increasing generation of diverse waste, environmental pollution, and escalating energy consumption drive the quest for innovative approaches to utilize waste alongside fuel and value-added materials production. Additionally, amidst the current political and energy turmoil stemming from global instability, exploring alternative energy sources is imperative. Harnessing renewable fuels and waste for energy production is vital environmentally and economically, serving as a response to the energy crisis.



FIGURES



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ELECTRIFICATION OF STEAM METHANE REFORMING

RESEARCH ABSTRACT

This review explores the advancements and potential of Steam Methane Reforming (SMR) technology, focusing on the comparison between conventional SMR and its electrified counterpart, as well as the integration of membrane reactors. Conventional SMR has long been the primary method for hydrogen production, but electrified SMR presents opportunities for enhanced efficiency and reduced emissions through the utilization of renewable electricity sources. Additionally, membrane reactors offer advantages in terms of selective product separation and improved process economics. This review discusses the key principles, advantages, and challenges associated with each approach. Furthermore, it presents potential avenues for future research, emphasizing the need for advancements in catalyst development, membrane materials, and process integration to optimize the performance and sustainability of SMR technology.

FIGURES





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THERMAL MODELLING OF LARGE-SCALE LIQUID HYDROGEN TANKS

RESEARCH ABSTRACT

My thesis research is focused on thermal modelling of large-scale liquid hydrogen (LH₂) storage tanks which falls under the area of developing hydrogen supply chain. Currently, LH₂ is stored at 20K in vacuum jacketed vessels that are not scalable up to commercial tank sizes. Several engineering challenges need to be addressed at such low temperatures. Therefore, as a first step towards solving this challenge, design and modelling of the non-vacuum insulation system is needed. In cryogenic regime, physical properties of materials change dramatically. This poses numerical problems for state-of-the-art solvers that are used in industry. Thus, we have combined analytical and numerical techniques to reduce the problem complexity and solve it an order of magnitude faster than the existing packages. We have proposed a new pseudo-streamfunction that reduces the problem to two equations and then with spectral methods we construct the bifurcation diagrams. This work also covers a novel dual layer insulation design that provides a thinner insulation as compared to the single layer design.

FIGURES





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UNLOCKING ETHANOL'S POTENTIAL AS LIQUID ORGANIC HYDROGEN CARRIER: OPTIMIZING ETHYL ACETATE PRODUCTION FOR SUSTAINABLE HYDROGEN STORAGE AND TRANSPORT

RESEARCH ABSTRACT

This study explores ethanol's potential as a liquid organic hydrogen carrier (LOHC) for safe and efficient hydrogen storage and transport, offering a viable alternative to traditional methods like compressed or liquefied hydrogen. Ethanol, derived sustainably from biological sources, emerges as a promising candidate for LOHC production. By utilizing reversible chemical reactions, LOHC systems address key challenges in hydrogen storage, including safety concerns and infrastructure limitations. Ethanol's renewability and abundance make it particularly attractive for LOHC applications, aligning with sustainability objectives. Comparative analysis highlights the advantages of ethanol-derived ethyl acetate over other compounds like Acetaldehyde, emphasizing its low toxicity and reduced carcinogenicity. This underscores the importance of optimizing ethyl acetate selectivity during ethanol dehydrogenation. Ultimately, this research aims to enhance the efficiency and sustainability of ethanol-based LOHC systems by investigating catalytic mechanisms, particularly focusing on improving ethyl acetate selectivity through interfacial effects in Cu catalysts. Such advancements could significantly contribute to the feasibility and adoption of hydrogen storage and utilization technologies.

FIGURES



Figure 1: Volumetric vs Gravimetric hydrogen storage capability for various hydrogen carriers



Figure 2: Product distribution over different Cu Catalysts for Ethanol Dehydrogenation



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DEVELOPMENT OF FEMOO⁴ **TRANSITION METAL OXIDE ELECTROCATALYST TOWARDS OXYGEN EVOLUTION REACTION UNDER ALKALINE CONDITIONS**

RESEARCH ABSTRACT

Electrochemical water splitting emerges as a pivotal strategy for sustainable hydrogen energy production. Alkaline water electrolysis offers a facile pathway to yield pure hydrogen. However, the anodic oxygen evolution reaction (OER) poses a formidable challenge due to its intrinsically sluggish kinetics. Overcoming this hurdle demands efficient water oxidation electrocatalysts to mitigate overpotential and enhance overall efficiency. While state-of-the-art catalysts such as RuO and IrO excel in OER catalysis, their limited availability and high cost impede broader implementation. The bimetallic oxides of Fe and Mo possess such an electronic structure that the surface adsorptiondesorption kinetics of the reaction becomes optimum. Utilizing a hydrothermal synthesis method, FeMoO, supported over Nickel Foam (NF) substrate was synthesized. Characterization techniques including Scanning Electron Microscopy (SEM) revealed nanosheets agglomerated nanospheres of the FeMoO, moieties which provide a large surface area for the OER. Cyclic voltammetry measurements present an overpotential of 228 and 315 mV at 10 and 1000 mA/cm2 respectively which is much lower than recently reported a noble metal oxide electrocatalyst like IrO2/NF (290 mV at 10 mA/cm2) and RuO_/NF (263 mV at 50 mA/cm2). These findings underscore the potential of FeMoO_ as a cost-effective and promising candidate for advancing the field of water oxidation in electrochemical water splitting.

FIGURES





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