

## Session 1

### **Abstract (#19413)**

**Title:** Recycling Polymers to Chemicals

**Authors:** Arthur Garforth, Aleksander Tedstone, Abdulrahman bin Jumah, Isaac Campbell and Chris Hardacre

**Manchester University**

Polymers are extremely stable and decomposition in a landfill occurs over extended periods, with the introduction of more stringent environmental regulation, rising landfill costs and the drive towards a circular economy, there is an increasing need to redirect polymer waste from landfill/energy recovery towards enhanced recovery of the raw materials. The two main routes for the recycling of polymer waste are mechanical and chemical. The most widespread approach to chemical recycling is pyrolysis (or cracking), however, this process requires high operating temperatures (typically 500°C – 900°C) with a subsequent large adiabatic temperature drop across the reactor (fixed bed or fluidised), which combined with catalyst deactivation, results in significant processing issues.

A more energy neutral option is that of hydrocracking, which offers the potential for the selective recovery of useful chemical fractions but is also tolerant of the presence of heteroatoms such as bromine and chlorine. The hydrocracking of PE and PP, mixed polyolefin blends and mechanical recycled PP from scrapped cars were carried out using in a 300 cm<sup>3</sup> stainless steel stirred autoclave (Parr, USA) using zeolite catalysts (1.5g, typically loaded with 1 wt. % Pt). The key parameters investigated were mixing, temperature (200°C–350°C) and hydrogen pressure (300 – 1000 psig).

As expected, increasing T increased lighter product yield and reducing hydrogen pressure increased coke yield and decreased catalytic activity. Typically all polymers and blends tested turned the waste into gas (C3-C4) and naphtha fractions (C5 – C12) with a high proportion of branched isomers. The mechanically recycled PP gave lower conversions however, the product range was typically C4-C6. Using a model compound, this research also demonstrated that mildly exothermic hydrocracking can be carried out at significantly shorter reaction times (typically 5 min.), making continuous processing of polymer waste a possibility.

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**Abstract (#19393)****Title:** Design of Sustainable Packaging using Simulation Based Optimization**Authors:** Abdul Rahim Arafath, Raghavendra Janiwarad, Bhaskar Patham**SABIC**

Packaging plays a critical role in the safe and effective delivery of goods. Plastic packaging faces up to increasing criticism due to their significant contribution to community's solid-waste burden. The new environment law around the globe and consumer pressure are prompting manufacturers to rethink and optimize the design of plastic packaging. Today's manufacturers cannot afford to waste a gram or a micron on non-essential material in the packaging and shipment of their products.

That is one reason major manufacturers of packaged goods are turning to computer-aided engineering (CAE) techniques to simulate and optimize the shape, size, weight and performance of packaging without sacrificing performance and durability.

This work explore the usage of simulation based optimization in the earliest stage of design process to develop sustainable plastic packaging solutions.

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**Abstract (#19277)****Title:** Experiences from Management of Ageing & Life Extension of Subsea flexible Pipes and Marine Hoses**Authors:** Konstantinos Vatopoulos.**Saudi Aramco**

Flexible pipes are used extensively in the offshore oil and gas industry. The trend for utilizing these technologies is increased due to the ever-increasing water depths and dynamic offloading challenges. The design, manufacture and deployment of flexible pipes has been developed extensively, however many challenges in integrity of pipelines still exist.

The paper provides an overview of best practices on how to better manage these systems and address their life extension. The paper covers available standards, guides and publications for pipeline integrity in flexible pipes and hoses. It describes different classifications of flexible pipe and hose construction, advantages over steel risers, as well as a description of the materials, manufacturing methodology, quality assurance and application examples for un-bonded and bonded pipe and systems. The paper then makes an overview of currently used inspection and monitoring techniques for these systems. Life assessment methods, assessment models, environmental data, degradation mechanisms and reuse considerations are described. Finally, the analytical techniques used to describe degradation and model life extension are described, and typical operational considerations through lessons learned are summarised.

The products covered within this paper are evolving constantly. This is driven by many factors:

- Operators requesting the product to work in more demanding projects (water depths, higher dynamic loading);
- Manufacturing methodologies changing; New materials being developed and older materials being modified;
- Requirements to reduce product costs to remain a competitive offshore solution;
- Experience in all aspects of the products increasing due to the huge rise of product deployment;
- Recovery and dissection of operational pipelines to learn about degradation and performance in addition to failure modes;
- Lessons learnt being shared across the industry;
- Challenges to the design guidelines and global specifications;
- New and more robust analytical methods coupled with more refined metocean data;
- A desire and necessity to extend life to remain competitive in a challenging oil and gas market;

This paper aims to assist integrity engineering of offshore flexible pipe and hoses with a specific focus on the non-metallic (NM) components of these structures. Current industry ageing and life assessment procedures do not take full account of the degradation potential of NM materials, but tend to concentrate on metallic aspects and conventionally understood liner function degradation mechanisms. As design guidelines are challenged and inspection techniques are improved within the metallic sections of a flexible pipe or hose, there is a greater need to ensure that the non-metallic components are also assessed appropriately.

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### **Abstract (#19272)**

**Title:** Life Cycle Assessment for Produced Water in Oil and Gas operations

**Authors:** E. Kremleva,

**Aramco Overseas BV**

Produced water represents a significant waste stream from oil and gas operations. The successful management strategy involves primary separation from oil, gas and solids, transportation from the field to water treatment facilities, and series of treatment technologies to bring the water quality to acceptable level depending on the final destination for water deposition (surface discharge, deep well injection, use in the oil and gas operations, drinking purpose etc.).

Several attempts were undertaken to evaluate oil field produced water treatment and disposal options for it through a Life Cycle Assessment (LCA) methodology, but until now, there is no clear understanding

of the whole system performance and comparative benchmark of produced water treatment technologies.

The focus here is on analysis of different approaches for produced water treatment and disposal and comparison of them on the basis of their LCA performance. The technical and environmental performance of different technologies, energy and process efficiency as well as potential impacts on health and environment have been evaluated. In this study, technical data from existing paths of produced water and its utilization strategies were acquired, and a quantitative environmental assessment by means of holistic tools of sustainable engineering were developed.

The results of the study offer a valuable insight into LCA methodology, provide arguments for the discussions on which treatment option and utilization will be the most beneficial. Appropriate design of produced water treatment systems in the oil and gas industry may be an effective action to reduce the environmental impact of the industry and improve its social acceptance. "

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## Session 2

### **Abstract (#19412)**

**Title:** Analysis and optimization of multi-path CCU system using a computer-aided tool

**Authors:** Wonsuk Chung, Ali S. Al-Hunaidy, Hasan Imran, Jay H. Lee

**KAIST**

Carbon capture and utilization (CCU), a promising solution for mitigation of global climate change, usually contains multiple carbon sources and multiple products, resulting in numerous candidate CCU pathways. Accordingly, a systemic analysis is essential to identify feasible or most attractive pathways. We have developed a computer-aided tool with graphic user interface named as Aramco-KAIST tool for CO<sub>2</sub> capture and conversion (ArKaTAC3) that help the user model, analyze and optimize the CCU superstructure. This software embeds three functions: (1) nonlinear shortcut models for the capture processes, (2) techno-economic and life cycle inventory (LCI) data for capture and conversion processes, (3) ability to handle exogenous uncertainties such as fuel price change and energy switch from fossil-fuel based to renewable, and (4) implementation of an open-source nonlinear programming (NLP) optimizer. A CCU superstructure that captures carbon from refinery off-gases is analyzed and optimized under provided demands for the products. The computer-aided tool successfully optimized the multi-objective problem with profitability and carbon reduction criteria under varying circumstances.

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### **Abstract (#19388)**

**Title:** Intermediate Temperature CO<sub>2</sub> Capture: a New Promising Pathway for Future Low-Cost CCUS

**Authors:** Takuya Harada, Cameron Halliday, Aqil Jamal, Alan Hatton.

**MIT**

The establishment of low-cost commercially viable carbon capture, utilization and storage (CCUS) platform is an urgent global challenge for the realization of sustainable future society while keeping the utilization of fossil fuels as a stable resource of energy and materials. In this presentation, we demonstrate our recent progress on the developments of advanced sorbents and the processes for CO<sub>2</sub> capture operating at intermediate temperatures in the range of 200-700 °C, and discuss the advantages of “intermediate temperature CO<sub>2</sub> capture” for the implementation of future low-cost CCUS systems.

First, we review our strategies to realize high performance metal oxide-based CO<sub>2</sub> adsorbents. Here, we demonstrate two successful approaches; the enhancement of reaction kinetics of CO<sub>2</sub> adsorption on the basic metal oxides by a functional surface coating with molten ionic salts, and the control of uptake

equilibrium by the design of new metal oxides composites. Next, we present a new conception to realize thermally stable fluidic sorbents for the establishment of a low-cost continuous CO<sub>2</sub> capture systems, and propose a colloidal dispersion of metal oxide nanoparticles in molten salts as a promising new sorbent, We further examine the performances of these new sorbents in practical CO<sub>2</sub> capture systems by the process model analysis. Energy cost of intermediate temperature CO<sub>2</sub> capture, efficiency of H<sub>2</sub>/CO<sub>2</sub> separation for pre-combustion process will be examined based on the comparison of experimental and model simulation results. In closing, we will comment on the future perspective of CCUS pervasion under the accelerating innovations of advanced CO<sub>2</sub> capture technologies.

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**Abstract (#19507)**

**Title:** Efforts for CO<sub>2</sub> Sequestration, Metal nanoparticles, Nanocomposite and Membrane

**Authors:** Nezar H Khdayr

**KACST**

Carbon dioxide has a significant impact on climate change. In this work, the Carbon dioxide uptake using metal nanoparticles will be addressed. Amorphous silica was decorated with metal nanoparticles and employed for CO<sub>2</sub> capture. The surface was functionalized using N-[3-(trimethoxysilyl)propyl]ethylenediamine (PEDA) as coupling agents, followed by complexation with metal ions to produce metal ion–ethylenediamine–silica nanocomposites. Finally, the metal ions were converted to metal nanoparticles using redox chemistry. Further effort was carried out by implanted modified silica in the PVDF-membrane to give more flexibility of designing the CO<sub>2</sub> Uptake device. This process formed uniform metal nanoparticles on the silica surface. The metal nanoparticle grafted silica composites were characterized by a number of techniques such as FTIR spectroscopy, thermogravimetric analysis, element analysis (CHN), X-ray diffraction, energy dispersive X-ray spectroscopy (EDX), surface area analysis, scanning transmission electron microscopy and gas analysis system.

Cu and Ag nanoparticles showed a uniform distribution into the silica surface. The diameter of metal nanoparticles was around 10 nm and the capacity of carbon dioxide for nanocomposites was significantly increased by 100%. Silica-Cu nanoparticles show the optimum capacity of 0.52 mmol g<sup>-1</sup>. This method will touch a new horizon of cheap catalyst for the synthesis of a variety of metal nanocomposites for their probable applications in greenhouse gas uptake and reuse.

**Abstract** (#19454)**Title:** Catalytic Non-Redox Carbon Dioxide Fixation in Cyclic Carbonates**Authors:** Cafer T. Yavuz Saravanan Subramanian, Doyun Kim, Thien Nguyen, Mousumi Garai, Wonki Lim**KAIST**

To make cycloaddition of CO<sub>2</sub> to epoxides a viable non-redox CO<sub>2</sub> fixation path, it is crucial to develop active, stable, selective, metal-free, reusable, and cost-effective catalysts. We recently reported several new structures based on imidazolinium and bisimidazolium functionalities that are synthesized from widely available chemicals. The porous catalysts exhibit quantitative conversion and selectivity for a range of substrates under ambient conditions and without the need for co-catalysts, metals, solvent, or pressure. They're easily recyclable and demonstrated to retain complete retention of activity for over 15 cycles. Moreover, they're scalable to at least a kg scale. We determined the reaction mechanisms using Quantum Mechanics (Density Functional Theory) showing that it involves Nucleophilic attack Driven Epoxide Ring opening (ND-ERO). This contrasts with the commonly assumed mechanism involving concerted addition of chemisorbed CO<sub>2</sub>.

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## Session 3

### **Abstract (#19341)**

**Title:** Photocatalytic CO<sub>2</sub> Conversion Using Cu-Based Cocatalysts with Varying Surface Treatments

**Authors:** Doh C. Lee, Gwuimin Kim, Ilsong Lee, Pan Lu, Sunil Jeong.

### **KAIST**

Ultimate utilization of photocatalysts for the CO<sub>2</sub> reduction would require the microscopic understanding of reduction mechanism and design of photocatalytic materials that can maximize the conversion yield. In this study, we prepared hetero-nanostructure semiconductors that can facilitate photocatalytic efficiency and selectivity of CO<sub>2</sub> reduction. In particular, we focus on the use of Cu-based cocatalysts on photocatalytic particles and their design in terms of heterostructures and surface ligands. Photocatalytic activity improves when the photogenerated electrons and holes become available to participate in reduction and oxidation on the surface, respectively. Prolonged electron-hole recombination time and heterostructures with both reduction and oxidation sites available on the surface are deemed to enhance photocatalytic activity. We expanded the idea into the design of photoelectrochemical cells, in which electrodes are constructed in a way that photogenerated electron and hole are likewise easily dissociated. A principle that underlies the design strategy is to synthesize nano-sized junctions with electron-hole separation, with the structure of “open” geometry, such as tetrapods. In addition, we investigated the effect of surface facets of various transition metal cocatalysts. In this presentation, we will discuss the effect of alloys, cocatalyst size, and surface facets on the conversion yield and selectivity of the reduction.

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### **Abstract (#19600)**

**Title:** Cascaded Electrolysis to Optimise The Direct Electrochemical Conversion of CO<sub>2</sub> to C<sub>2</sub>/C<sub>3</sub> Hydrocarbons

**Authors:** Maximilian Fleischer, Sofia Romero, Christian Scherrer, Kai-Olaf Hinrichsen.

### **Siemens AG**

The cheap electricity available from photovoltaics in sun rich countries might be increasingly used to supply raw materials for the of the chemical and petrochemical industry. When CO<sub>2</sub> from exhaust gases or captured from air is used, these molecules bear a green character that can have an influence on their sales revenue.

Since solar energy can be cheap but needs to be financed, strong research and industrial R&D is needed to optimize the required technologies for best energy efficiency. Water electrolysis to H<sub>2</sub> that needs to be combined captured of CO<sub>2</sub> in thermochemical reactions is the first entry point of electricity to the



chemical sector. The optimization of these processes is ongoing [1] with a typical energy efficiency from electricity to energy in the chemical bonds being currently about 50 %.

In contrast to this, the direct electrochemical CO<sub>2</sub> conversion comes up, promising even better potential energy efficiencies, since no high-temperature thermochemical conversion is used for the CO<sub>2</sub> activation. The reduction of the CO<sub>2</sub> to CO works in aqueous media and for the delivery of CO or SynGas is already in the scale up [2]. The direct reduction of the CO<sub>2</sub> to hydrocarbons would be preferred but proved to be very difficult in worldwide research. We investigate the approach of a cascaded electrolysis from CO<sub>2</sub> over the intermediate CO to C<sub>2</sub>/C<sub>3</sub> hydrocarbons. This separation of the process has the potential of separately optimized process conditions. Ag catalyst in neutral/acidic electrolyte can be used in the first and Cu catalyst stabilized by alkaline electrolyte can be used for the second step. Using CO to get the C<sub>2</sub>/C<sub>3</sub> hydrocarbons allows higher selectivities reaching over 75% faraday efficiency [3]. To show that this idea works in practice we build and will present the first integrated two-step electrolyzer device. It is working with industrially relevant current densities of >> 100mA/cm<sup>2</sup> at electrode sizes of 10cm<sup>2</sup> and is operated over days in stable condition. Even without further optimization 60+% faraday selectivity to C<sub>2</sub>/C<sub>3</sub> is shownreached.

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**Abstract (#19323)**

**Title:** Non-Reductive Catalytic Conversion of Carbon Dioxide to Organic Carbonates and Carbamates

**Authors:** Keiichi Tomishige

**Tohoku University**

Catalytic conversion of carbon dioxide into useful compounds can contribute to the construction of future sustainable society. Reaction of CO<sub>2</sub> with alcohols and amines to corresponding carbonates and carbamates is non-reductive conversion of CO<sub>2</sub>, and it is found that CeO<sub>2</sub> is an effective heterogeneous catalyst for these reactions. The conversion and yield of products is seriously limited by the reaction equilibrium, for example, in the reactions of CO<sub>2</sub> with alcohols and anilines. The combination of these reactions with the hydration of 2-cyanopyridine or 2-furonitrile, which is also catalyzed by CeO<sub>2</sub>, enabled very high conversion and yield of the target products. It is also reported that the interaction between 2-cyanopyridine and CeO<sub>2</sub> surface gives very strong base sites which plays an important role on the activation of alcohols. In the presentation, the direct polymerization of CO<sub>2</sub> and alpha,omega-diols to polycarbonatediols from catalyzed by CeO<sub>2</sub> using nitriles as a dehydrating agent, which have been used for the production of polyurethanes. Recently, it is found that the formation of polycarbonates with higher molecular weight in the CeO<sub>2</sub> + 2-furonitrile catalyst system than the case of CeO<sub>2</sub> + 2-cyanopyridine, and this behavior is discussed on the kinetic analysis and DFT calculations. In addition, the direct catalytic synthesis of carbamates from CO<sub>2</sub>, anilines and methanol was achieved by controlling both the reaction equilibrium and the reactivity of the three components. The combination of CeO<sub>2</sub> and 2-cyanopyridine was an effective catalyst, providing various carbamates including N-arylcarbamates in high selectivities.

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**Abstract (#19526)**

**Title:** A Methodology for Developing Effective Approaches for CO<sub>2</sub> Utilisation

**Authors:** Tony Picaro

**Aramco Overseas Company B.V.**

The field of CO<sub>2</sub> utilisation is seeing an ever increasing breadth of activities from diverse organisations (industrial, government, academic) focusing on no longer treating CO<sub>2</sub> as a waste product, but as a valuable resource. CO<sub>2</sub> utilisation is a broad term that covers a variety of processes that can transform carbon dioxide into a variety of value added products such as chemical products, synthetic fuels, and building materials. There are a number of key approaches for utilising CO<sub>2</sub> which can be divided into the following key categories:

- Catalytic
- Electrochemical
- Microbial
- Photosynthetic
- Photocatalytic
- Mineralisation

There is no single, universally applicable pathway for utilizing CO<sub>2</sub> as there are many factors which need to be considered, including the type of industry, its location, as well as many other constraints (political, social, etc.). Consequently, one or more technologies may fit better than others. An approach that integrates different methods may be the most practical solution for many applications.

It is estimated that CO<sub>2</sub> utilisation technologies can potentially reduce CO<sub>2</sub> emissions by about 10% of the world's current annual anthropological emissions. This suggest that the potential impact of CO<sub>2</sub> utilisation may be limited as to whether it can become an accepted and/or effective approach by which future utilisation of fossil fuel resources can be achieved in a more environmentally friendly way that helps reduce global warming.

However, CO<sub>2</sub> utilisation can play a part in the greater effort to open up the opportunity for pre- or post-combustion CCS (carbon capture and storage) technologies to give value-added products that can in theory offset the costs of plant investment or even make the process profitable.

CO<sub>2</sub> utilisation will be attractive if/when carbon dioxide is a cheaper source of carbon than other feedstocks (fossil fuels etc.) to make plastics, chemicals, etc. Some of the key issues which need to be addressed in order for CO<sub>2</sub> utilisation to be deployed, include:

- Carbon capture costs are critical for commercial deployment
- What CO<sub>2</sub> purity is required for utilisation?
- What are the costs to transform CO<sub>2</sub>?

- What to transform CO<sub>2</sub> to, e.g. high value products (chemicals) or low value products (fuels)?

An assessment of a number of novel and innovative approaches to valorising CO<sub>2</sub> are described in order to present a methodology for selecting potential approaches for developing effective CO<sub>2</sub> utilisation processes that are suitable for deployment.

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## Session 4

### **Abstract (#19376)**

**Title:** The Impact of Limestone Properties on Calcium Looping at Heavy Fuel Oil-Fired Power Plants

**Authors:** Sally L. Homsy, Robert W. Dibble

### **KAUST**

Eliminating emissions from the power sector requires investment in a portfolio of technologies, including carbon capture and sequestration (CCS). The associated economic penalty is reduced by implementing CCS at power plants firing low value fuels such as heavy fuel oil (HFO). HFO is a regionally available, low cost, highly sulfurous, residual petroleum fuel. Although CCS implementation at coal-fired plants has been studied extensively, literature on CCS implementation at HFO-fired power plants is scarce. Calcium looping (CaL) is an advanced post-combustion CO<sub>2</sub> capture technology that utilizes limestone derived calcium oxide as a CO<sub>2</sub> sorbent. Since CaO sulfation occurs at typical process conditions, CaL can simultaneously concentrate CO<sub>2</sub> and capture SO<sub>2</sub> from HFO flue gas. CaL typically utilizes two interconnected fluidized beds to cycle between CaO carbonation and calcium carbonate calcination. The energy penalty associated with CaL implementation at HFO-fired power plants can be reduced by optimizing the process heat balance while accounting for HFO flue gas composition and limestone performance. Reasonable limits on operating parameters for CaL implementation at HFO-fired power plants are calculated and discussed in this work. Two structurally distinct limestones from different geological regions are considered: (1) Riyadh limestone, and (2) Saabar limestone.

Bubbling fluidized bed (BFB) reactors equipped with effluent line sampling for continuous CO<sub>2</sub>, SO<sub>2</sub>, and O<sub>2</sub> gas analysis were used to determine Riyadh and Saabar sorbent capture performance at relevant conditions. Limestone samples were cycled between calcination and carbonation in the presence of: (1) steam, (2) both steam and SO<sub>2</sub>. Relative limestone attrition, sintering, and deactivation rates were assessed. Samples at different stages of activity ( $X_{max} = 0.6, 0.3$  and  $0.1$ ) were collected and used to examine the influence of sorbent cycling and CaSO<sub>4</sub> content on CO<sub>2</sub> and SO<sub>2</sub> co-capture from synthetic HFO flue gas during carbonation. A thermogravimetric analyzer was used to assess limestone deactivation rates due to cycling at different looping rates in relevant gas atmospheres. Using this experimental data, CO<sub>2</sub> and SO<sub>2</sub> capture rates and limestone deactivation rates were estimated for a range of operating conditions relevant for CaL implementation at HFO-fired power plants. Process mass and heat balances were solved to determine preferred CaL system operating conditions for each of the limestones. Riyadh limestone utilization was found to be advantageous when employing a relatively high make-up ratio and high  $X_{max}$ , while Saabar limestone is slightly more suitable when a high looping ratio, low  $X_{max}$ , and high carbonator bed inventory are maintained.

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### **Abstract (#19395)**

**Title:** A Diesel-Driven Solid Oxide Fuel Cell System for Auxiliary Power Unit Applications

**Authors:** Joongmyeon Bae, Minseok Bae, Sai P. Katikaneni

#### **KAIST**

A diesel-driven solid oxide fuel cell (SOFC) system for auxiliary power unit applications has been designed with collaborative research between Saudi Aramco and Korea Advanced Institute of Science and Technology (KAIST). An auxiliary power unit can be used to produce electricity at remote regions such as gas wells, islands, and also heavy-duty vehicles. Fuel cell-based auxiliary power units are promising to generate electricity with hydrogen-based fuels without noise, and pollutants. Diesel can be utilized as a source of hydrogen-rich gas for operating fuel cells, with its high energy density and versatility. A diesel autothermal reformer has been introduced to convert diesel to hydrogen, and the produced hydrogen-rich gas is provided to SOFC stack to generate electricity. With the integration of the reformer and SOFC stack, an auxiliary power unit with one-kilowatt power output has been designed. Structured catalysts were introduced for the diesel reformer to ensure the mechanical strength of the component. During the development of the diesel reformer, a long-term test of 2,000 hours for the catalyst component was conducted to ensure its catalytic stability.

The SOFC stack operates with an operating temperature of around 700 deg C, and the thermal stability of the stack can determine overall system start-up time. Two versions of the integrated fuel cell system were designed with different assumptions for the start-up time of the SOFC stack. The first version of the system assumed slow start-up of the SOFC stack, so the design for the heat network of the system was limited to ensure stable start-up of the SOFC stack. However, the start-up time of the fuel cell system could be shortened if the fuel cell stack has enough thermal stability that can sustain the fast heat-up process. Therefore, the system configuration can also be modified at the improved version by using external heat sources during the start-up process. In result, shorter start-up time and simplified start-up process were obtained with the enhanced design of the fuel cell system.

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#### **Abstract (#19489)**

**Title:** Marketable prospects of microbial fuel cell for clean energy generation and wastewater treatment

**Authors:** Mohammad Salim Akhter

#### **University of Bahrain**

Microbial fuel cells (MFCs) are bioelectrochemical devices, which produce electrical energy from wastewater through degradation of biodegradable organic substrates. The use of MFCs for energy generation from wastewater biofuels through electrochemically active bacteria as biocatalysts has been widely accepted in the recent past. The ability of MFCs to utilize organic compounds present in wastewater as anodic fuels suggests their feasibility as bioelectrochemical systems for producing power and debasing pollution. The power output of MFCs depends upon the electrode material, pH of the medium, temperature, internal and external impedance values, as well as redox potentials of cathodic and anodic chambers. The findings of the present work highlight the importance of tuning these

parameters for improving energy generation efficiency of MFCs. As every technology has associated merits and demerits, so to avoid offering details of only success stories, here an effort has been made to critically discuss the recent progress and challenges in the practical applicability of MFC as energy source and water purification technology. This work is expected to provide critical information to engineers and environmental stakeholders to invest on upgrading MFC technology for ensuring zero carbon based energy generation and safeguarding human life from water toxins.

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**Abstract (#19274)**

**Title:** Simulation Driven Clean Fuel Design

**Authors:** S. Mani Sarathy

**KAUST**

Design of chemical processes requires fundamental knowledge of how molecular structure of reactants affects product distribution and energy release. This research combines state-of-the-art comprehensive kinetic models together with high fidelity experimental measurements to study complex chemical processes. The research involves the development of large databases of chemical reaction pathways with associated kinetic rate parameters, as well as thermochemical and transport properties for all reactant, intermediate, and product species. First, we apply a range of high-resolution analytical techniques to characterize complex mixtures at the molecular level, and then surrogate mixtures with a limited number of components are designed to match important target properties. Detailed reaction pathways are written for the surrogate components to simulate chemical reactions at conditions relevant to real-world applications. The art of assigning rate constants using chemical intuition and quantum chemical modeling are important parts of my research. The determination of thermochemical and transport properties is achieved using both molecular modeling tools and empirical methods. The comprehensive models are validated against data from well-defined experimental configurations, such as zero-dimensional and one-dimensional reacting flows in which fluid physics can be modeled exactly. Engineers utilize my tools to design better engines and fuels, study urban air quality, and simulate catalytic reactors.

## Session 5

### **Abstract (#19511)**

**Title:** Leading-Edge Mirrorless Solar Thermal Panels Reduce Running Costs and Clean Upstream Oil & Gas Image

**Authors:** Jonathan Koifman, Piero Abbate

### **TVP Solar**

At Saudi Aramco's Qurayyah utility plant, an innovative solar thermal field cuts liquid fuel use. TVP Solar, a Swiss manufacturer of unique evacuated solar thermal flat plates, supplies 164°C without mirrors to preheat utility steam boiler feedwater. Covering up to 50% of daily sensible heat thermal energy need, over 132'000 litres of diesel per year are saved and 345 tonnes of CO<sub>2</sub> cut.

Considering the energy intensity of oil and gas operations, O&G players focus on process optimization, energy efficiency, OPEX reduction, and minimisation of fuel use to reduce their energy and carbon intensity. The Qurayyah solar deployment proves that solar thermal operating between 65°C and 180°C can achieve these targets and also be applied in other O&G facilities such as GOSPs desalter and separation fluid heating, boiler pre-heating, amine regeneration in gas sweeteners and carbon capture, EOR (for shallow wells).

Aramco's leading-edge high-vacuum non-concentrating solar thermal solution installation offers unique advantages: (i) continuous daytime operation, unattended and automated; (ii) consistent yearly energy supply, even in wintertime with low-azimuth sun trajectory and high diffuse light conditions; (iii) no need for cleaning.

Historically, solar thermal supplying over 100°C required mirror-based tracking, either parabolic trough or Fresnel collectors. These concentrators, due to optical physics constraints, do not capture diffuse light (critical in desert environments, or when dust accumulates on the collector), requiring daily water-based precision cleaning. The panels are SolarKeymark™-certified as the best collectors to capture and transform both direct and diffuse light up to 200°C, uniquely not requiring cleaning.

The 1'020 m<sup>2</sup> solar field in Qurayyah heats the feedwater from 93°C to 164°C of a 1.8MW thermal diesel boiler, serving 48.5% of the yearly sensible heat energy load. The solar system supplies over 4,300 MMBtu/year, up to 12 hours per day, reducing burning of liquid fuel.

When scaling up a solar thermal field to full utility scale, the anticipated cost of solar thermal energy can drop to below 4 USD/MMBtu. This solar solution is extremely competitive for process optimization, CO<sub>2</sub> cutting, and OPEX savings.

**Abstract (#19259)**

**Title:** Solar Energy Storage Using Shape-Stabilized Phase Change Materials: MgO and Mg(OH)<sub>2</sub> Containing Polyethylene Glycol.

**Authors:** Md. Hasan Zahir.

**King Fahd University of Petrol**

Organic and inorganic materials can store ambient heat and release it when necessary by temperature-controlled phase change. This process offers an ideal method of efficient solar energy management and utilization. Phase change materials (PCMs) are important commercially available heat storage materials of high latent heat density with a capacity to maintain a constant temperature during heat release. PCMs can be utilized in many fields, including smart housing, solar energy utilization, temperature-controlled greenhouses, temperature-regulating textiles, and heat management in electronics. In this study, heat energy storage systems were fabricated with the impregnation method by using MgO and Mg(OH)<sub>2</sub> as supporting materials and polyethylene glycol (PEG-6000) as the functional phase. MgO and Mg(OH)<sub>2</sub> were synthesized from the salt Mg(NO<sub>3</sub>)-6H<sub>2</sub>O by performing hydrothermal reactions with various types of precipitating agents. The precipitating agents were NaOH, KOH, NH<sub>3</sub>, NH<sub>3</sub> with pamoic acid (PA), or (NH<sub>4</sub>)<sub>2</sub>CO<sub>3</sub>. Our results show that the selection of the precipitating agent has a significant impact on the crystallite structure, size, and shape of the final products. Of the precipitating agents tested, only NaOH and NH<sub>3</sub> with PA produce single-phase Mg(OH)<sub>2</sub> as the as-synthesized product. Pore size distribution analyses revealed that the surfaces of the as-synthesized MgO have a slit-like pore structure with a broad type pore size distribution whereas the as-synthesized Mg(OH)<sub>2</sub> has a mesoporous structure with a narrow pore size distribution; this structure was found to enhance the latent heat of the PCM as well as to mitigate supercooling. The PEG/Mg(OH)<sub>2</sub> PCM also exhibits reproducible behavior over a large number of thermal cycles. The heat storage capability, microstructure, and interactions with the PEG/Mg(OH)<sub>2</sub> composite were characterized using DSC, SEM imaging, FTIR, Raman spectroscopy, and TGA. The liquid PEG was found to be stabilized within the porous matrix. The thermal conductivity of composite PCMs was also increased. A viable shape-stabilized composite PCM system for use in thermal energy storage was developed.

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**Abstract (#19330)**

**Title:** ZnSnN<sub>2</sub> Semiconductor Thin Film Deposited by PVD Magnetron Sputtering for Photovoltaics Applications

**Authors:** F. Alnjiman A, almoshawah, A. Alodhyay, S. Diliberto, S. Bruyère, J. Ghanbaja, P. Miska, H. Albrithin, J.F. Pierson

**King Saud University**

Nitride semiconductor materials have attracted considerable interest for solar energy application and high speed electronics. More especially, Zn-IV-N<sub>2</sub> is a new family of nitride semiconductor materials with



great potential of applications for solar materials [1]. According to the literature data, ZnSnN<sub>2</sub> may crystallize in several structures : orthorhombic Pna2<sub>1</sub>, orthorhombic Pmc2<sub>1</sub>, hexagonal P6<sub>3</sub>mc, or monoclinic P2<sub>1</sub>. It is hard to determine the structure and the lattice parameter by XRD due to the preferred orientation of our sputtered films.

This work presents the development of ZnSnN<sub>2</sub> thin films by reactive co-sputtering using zinc and tin metallic targets. The stoichiometry of the films was controlled by optimizing operating parameters such as the target voltage, the nitrogen partial pressure or the total pressure. The structure of the films was studied by X-ray diffraction. The films show a highly crystallization level and a strong preferred orientation in the [001] direction, with this texture it was hard to investigate the structure by XRD diffraction. The microstructure was observed by transmission electron microscopy. The selected area electron diffraction (SAED) pattern shows the growth direction of thin film of ZnSnN<sub>2</sub>. The results show that both monoclinic and orthorhombic structures can be excluded. Thus, our films crystallize in a hexagonal structure. Mössbauer spectrometry have been used to characterize the chemical environment on tin atom. Zinc tin nitride films exhibit an electron mobility at room temperature close to  $3.8 \times 10^{18} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and an optical band gap of 1.8 eV as measured independently from UV–visible spectrometry and ellipsometry[2].

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## Session 6

### **Abstract (#19282)**

**Title:** Nanocellulose from Date-Palm Trees. Phoenix Dactylifera L

**Authors:** Abdulrahman G. Alhamzani

**Imam Muhammad S University**

Cellulosic Natural fibers are naturally occurring hydrophilic polymer. They are the main substance that makes up plant cell walls and contributes to the physical stability of the cells. Nowadays, there is an increasing demand for more sustainable and renewable materials, and researchers exhibit in utilizing natural fibers for several applications due to their high specific properties. In this presentation, an Eco-friendly approach to prepare nanocellulose from the date-palm tree (Phoenix Dactylifera L.) wastes using a simple chemical treatment. Fibers could be extracted from different parts of the date palm, (e.g. trunks, fronds leaflets, sheath, and fruit bunch).

The main aim of this talk is to explore the preparation of Nanocellulose materials from local available agriculture waste (e.g. date palm trees) as a biomass resource, and optimize the conditions to obtain a high degree of purity of the product. Instead of discarding agriculture wastes into environment, they will be chemically converted into low-cost materials.

This proposed approach effectively reduced the need for multiple chemicals and offered more than 40% energy savings when compared to conventional multi-step processes in converting raw biomass into nanocellulose.

investigations and characterization of the obtained materials will be presented, such as X-Ray diffraction, FTIR, Scanning Electron Microscopic, and Thermogravimetric analysis TGA techniques. As well as, their potential applications for human beings will be explored.

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### **Abstract (#19321)**

**Title:** Crow Search Algorithm for Global Optimization of Papaya Oil Extraction Parameters

**Authors:** S. M. Zakir Hossain, S. Taher, A. Khan, N. Sultana, M.F. Irfan, S.A. Razzak, B. Haque

**University of Bahrain**

Papaya seed can be a reliable feedstock for producing valuable bioproducts (biodiesel, biolubricants, beauty product etc) due to its high oil content. This study aimed to investigate the effects of soxhlet extraction conditions (e.g., seed particle size and extortion time) on the yield of the oil from papaya seeds. Initially, Response Surface Methodology (RSM) with Central Composite Design (CCD) was applied for

predictive modeling of the yield of oil. Crow Search Algorithm (nature-motivated metaheuristic algorithm) coupled with RSM was utilized for global optimal solution. The global optimal point was found to be 6.5 h of extraction time and 0.65 mm of particle size with maximum yield of 29.96%. The predicted optimal set was also validated further by experimental yield of 31.1% with the variation of less than 5 % indicating the reliability of the extraction conditions. The extracted oil was characterized by GC-MS analysis

**Abstract (#19481)**

**Title:** Cryogenic Carbon Capture™ Applications and Results

**Authors:** Professor Larry BAXTER, Frankman, Andrew Baxter, Kyler Stitt, Chris Hoeger, Skyler Chamberlain, Eric Mansfield, Aaron Sayre, Stephanie Burt.

**King Abdullah University of Sc**

Sustainable Energy Solutions is commercializing a process called cryogenic carbon capture™ (CCC) that separates CO<sub>2</sub> from other gases in industrial processes. CCC finds application to:

1. Climate change mitigation when applied to flue gas treatments
2. Natural gas treating
3. EOR recirculation treating, and
4. Liquefied natural gas production, and
5. Energy Storage

The process cools the process stream to the point that CO<sub>2</sub> solidifies (usually desublimates), separates the solids from the fluid, and warms the products back to the initial temperature by cooling the incoming streams (see [www.sesinnovation.com](http://www.sesinnovation.com)). Detailed analyses by several third-parties indicate CCC consumes substantially less energy and costs significantly less than alternative processes. Alternative processes also require major upstream process modifications or replacement. By contrast, CCC requires no such modifications in that it is a bolt-on technology that can be added to any existing process with essentially no modifications to the existing assets. CCC also captures essentially all water, pollutants, and particulate from the process stream in the process of capturing CO<sub>2</sub>. In some embodiments, it enables grid-scale, rapidly responding energy storage capabilities. Different versions of the process apply to flue gas treating (oxidizing environments), syngas treatments (reducing, non-condensing environments), natural gas treating (reducing, condensing environments), EOR recirculation (very high CO<sub>2</sub> contents), and LNG production (very low CO<sub>2</sub> concentrations in the product).

This presentation describes CCC applications and presents results from laboratory and field tests.

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**Abstract (#19348)**

**Title:** CD-GO as an Effective Corrosion Inhibitor for Carbon Steel in Acidic Environment

**Authors:** Kabiru Haruna, Tawfik A. Saleh.

**KFUPM**

Cyclodextrin-based functionalized Graphene Oxide (CD-GO), was synthesized utilizing cost-effective waste graphite as a source for the production of graphene oxide. The obtained eco-friendly novel material, CD-GO, was characterized and evaluated for corrosion inhibition of X60 carbon steel in solutions of HCl at room temperature. The inhibition efficacy of the CD-GO material was evaluated by the use of the weight loss measurement as well as electrochemical techniques. The findings from both were in excellent agreements. CD-GO demonstrated high inhibition efficacy which enhances with increasing CD-GO concentrations. The SEM/EDX, FTIR, and UV-visible surface characterization analysis prove the adsorption of the protective film of CD-GO on the steel surface. The CD-GO materials were adsorbed on the surface of the steel via oxygen atoms of the CD-GO forming a CD-GO/metal complex on the steel surface. This work is of importance and has dual benefits; graphene oxide was prepared from waste graphite and converted into useful materials used to solve the corrosion problem

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