THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
The Gulf International Hotel, Kingdom of Bahrain
November 15 - 17, 2022

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR PROFESSOR OMAR YAGHI'S YOUNG RESEARCHER AWARD

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Correlation between of the structural and texture refinement of Nano-Sized ZSM-5 Zeolite and Plastic Waste Pyrolysis to Produce High Quality Carbon

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Abstract Ref Number from the website: **ID-6131**
Session: Materials: **Professor Omar Yaghi's Young Researcher Award**

ABSTRACT

This paper reports the purity, crystallinity percentage and crystal structure refinement of the synthesized nano-sized ZSM-5 zeolite with high crystallinity and yield by X-ray powder diffraction data and advanced Rietveld method. The zeolite exhibited better performance in light hydrocarbon aromatization reactions than conventional commercialized micro-sized zeolites. In the present study, Rietveld refinement with the generalized spherical harmonic description for correction of the preferred orientation in powder diffraction analysis (Alghamdi & Sitepu, 2018a&b; Ding, Sitepu & Alghamdi, 2018; Inan, Sitepu & Al-Ghamdi, 2019; Sitepu & Alghamdi, 2018, 2019; Ding *et al.*, 2021) for both crystal structure refinement and quantitative phase analysis are used to describe crystal structure and texture in all the X-ray powder diffraction data sets of the synthesized ZSM-5 powders (Al-Ghamdi *et al.*, 2022; Akpanudoh *et al.*, 2005; Chen & Manos, 2004; Manos *et al.*, 2001 & 2002). The results revealed that the structural refinement parameters obtained from the Rietveld refinement with the generalized spherical harmonic description, agreed well with the corresponding single crystal structure. In addition, the findings will correlate with the plastic waste pyrolysis over these well-characterized ZSM-5 catalysts at an optimum activation temperature to produce a char with high solid yield, minimize sulfur content and high amount of carbon. The exciting lab case study findings will be described in this paper and presented at the Professor Omar Yaghi's GCA-2022 Young Researchers Awards.

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Removal of Heavy Metals and Different Kinds of Anions from the Natural Water Through Graphene Nanostructured Materials

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Session: Materials: Materials for Environment and Wastewater Purification

ABSTRACT

In the present study, well-designed porous systems nanohybrids which convert two dimensional (2D) nanolayered structures to three-dimensional porous (3D) networks, sheets of graphene oxide GO and the nanolayers of layered double hydroxides (Zn-Al LDHs), and applied to act as effective dual-function adsorbents for removing both anions (accomplished by eliminating of 100% of hydrogen phosphate and bromide anions alongside with 80%–91% of sulfate, chloride, and fluoride anions) and heavy metals (by removing more than 80% of both cadmium and lead) from natural water, at the same time. A Quanta-chrome Nova sorption system was applied to perform these adsorption–desorption processes. Using the adsorption data, average pore radius, pore volume and specific surface area were assessed through the Brunauer–Emmett–Teller equation. The crystalline structures of GO, Zn-Al LDHs and the new nanocomposites were confirmed by XRD, FTIR, Raman spectroscopy. The morphology, shape surface and distribution of the samples were obtained directly using SEM and TEM. Materials surface area, pore volume, and pore size distribution were detected by BET.Removal efficiency of selected anions toward the different structures prepared: (a) W/V = 10 g/L, (b) W/V = 20 g/L, (c) W/V = 30 g/L.Removal efficiency of selected heavy metals (Cd &Pb) toward the different structures prepared: (a) W/V = 10 g/L, (b) W/V = 20 g/L, (c) W/V = 30 g/L

Introducing Cantellation Strategy for the Design of Mesoporous Zeolite-like Metal-Organic Frameworks: Zr-sod-ZMOFs as a case study

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ABSTRACT

In our continuous quest targeting materials with large pores featuring zeolitic topologies, a series of novel mesoporous Zr-MOFs showing the zeolitic sodalite (sod) topology is introduced for the first time.[1] These Zr-sod-ZMOFs have been designed and constructed following the molecular building blocks approach, unveiling the cantellation design strategy. Concretely, the organic linkers have been finely designed via derivation from enlarged tetrahedral building units approach, a prerequisite for a zeolite-like net. The two sod-ZMOFs in this work are highly porous frameworks with intricate truncated rhombic dodecahedron mesopores of ≈ 43 Å diameter and experimentally measured pore volume of 1.98 $cm^3 \cdot g^{-1}$, regarded as the highest reported exp. pore volume for ZMOFs based on

tetrahedral nodes [1]. Figure 1. Illustration of the bottom-up construction of Zr-sod-ZMOF-1 (center): (a) Organic and inorganic MBBs assemble through (b) the formation of triple bridges. (c) Each MBB connected to four others in a tetrahedral fashion. (d) Tetrahedral MBBs oriented in eclipsed fashion, with (e) a slight tilt characteristic of zeolites, allowing the overall formation of (f) the sodalite type cage.

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Novel Bifunctional, Trimetallic CuxZnyVO4 Microarchectures for Solar-Driven Water Splitting and Waste Water Remediation

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Session: Materials: Professor Omar Yaghi's Young Researcher Award

ABSTRACT

Herein, we report a novel and bifunctional β-$Cu_2V_2O_7$/$Zn_2V_2O_6$ (CZVO) heterojunction and their photocatalytic applications. The trimetallic CZVO demonstrates non-sacrificial photoresponse in the cases of; (1) photocatalytic degradation using methylene blue (MB) as a model dye, and (2) photoelectrochemical (PEC) water oxidation. After visible light exposure, CZVO-opt (1 wt.% CVO : 5 wt.% ZVO) demonstrates the highest photodegradation, which is 2.4-folds and 1.9-folds of neat CVO (2D layered) and ZVO (tablet-shaped nanoparticles), respectively. Similarly, the CZVO-opt photoanode delivers 1.78 mA cm^{-2} photocurrent density (Iph) at 1.23 VRHE, almost 3.11 and 1.55 times more than CVO (0.57 mA cm^{-2}) and ZVO (1.15 mA cm^{-2}) photoanodes, respectively with incident photon to current efficiency (IPCE320 nm) of 37.93 %. The significant improvement in the CZVO-opt performance can be attributed to the firm contact and uniform distribution of ZVO NPs over CVO interlayered nanosheets, which leads to type (I) heterojunction.

Preparation of low-cost metal oxide nanoparticle-modified carbon electrodes for enhanced oxygen evolution reaction

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Session: Materials: Professor Omar Yaghi's Young Researcher Award

ABSTRACT

Electrochemical/photoelectrochemical water oxidation i.e. oxygen evolution reaction (OER) is one of the most important approaches to convert renewable energy like solar energy to usable fuels. Generally, the OER is kinetically slow (i.e.it needs high overpotential) at the commonly employed electrode in both electrochemical or photoelectrochemical OER. As a result, the modification of the electrode with a suitable catalyst is needed to reduce the required energy and increase the rate of reaction. Therefore, several studies have been conducted with the objective of cost-effective catalyst preparation. Besides, most of the researchers have used high-cost materials as substrate electrodes such as gold and platinum. Here we will present cheap electrode materials (nano catalyst and substrate electrode) that we developed in our laboratory for electrochemical water oxidation. In this work, we used a low-cost porous carbon electrode (PCE) as a substrate for OER. We developed the filter paper-derived PCE (FPCE) by simply heating the normal filter papers in a nitrogen atmosphere in the tubular furnace. Then, we deposited very simply prepared NiO and Co3O4 NPs on the FPCE using a drop-drying method for OER. For the case of NiOx NPs preparation, we developed a novel method. Initially, we mixed carboxylic acid functionalized organic molecules (pamoic acid) and nickel precursors in an organic solvent. After removing the solvent, we heated dried reaction mass in an ambient atmosphere to obtain the monodisperse spherical NiOx NPs. Besides, we prepared Co3O4 NPs by direct thermal decomposition of commercially available cobalt precursor (Co(NO3)2·6H2O). We varied also thermal decomposition temperature to tune the morphological and electrochemical properties of the Co3O4NP. The used NPs (both NiOx and Co3O4) and the NPs-modified PCE were characterized in detail by various modern techniques such as scanning electron microscopy, transmission electron microscopy, Xray photoelectron spectroscopy, X-ray diffraction, Fourier transform infrared spectroscopy and thermogravimetric analysis. Both the NiOx and Co3O4 NPs -modified electrode showed significantly high electrocatalytic properties toward OER. In conclusion, the developed nanostructured-modified electrode materials are cheap and have high efficiency, which makes them attractive for water oxidation.

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR MATERIALS SYNTHESIS SESSION

6303

Materials -- Functional Material Synthesis and Characterization

DEHYDROGENATION OF FORMIC ACID MEDIATED BY A PHOSPHORUS–NITROGEN PN3P-MANGANESE PINCER COMPLEX: CATALYTIC PERFORMANCE AND MECHANISTIC INSIGHTS DEHYDROGENATION OF FORMIC ACID MEDIATED BY A PHOSPHORUS–NITROGEN PN3P-MANGANESE PINCER COMPLEX: CATALYTIC PERFORMANCE AND MECHANISTIC INSIGHTS

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Hydrogen is considered as a promising alternative to bridge the low-carbon energy to decarbonize the transportation sector which is still mostly relied on fossil fuel.[1] However, there is no viable process for hydrogen storage and transport since it costs an energy toll to compress or liquefy hydrogen. In this perspective, formic acid (FA), as liquid hydrogen carrier, has attracted much attention.[2] It has many desirable properties, such as low toxicity, low flammability and high volumetric capacity of 53 g H2/L to qualify as a suitable candidate. Although the FA dehydrogenation was first reported half a century ago, it is only the last decade that has witnessed a significant progress.[3] There has been a noteworthy development towards the catalysts based on noble metals. Alongside, exploration of 3d metals has achieved exciting results mainly with iron-based catalysts; however, manganese has not received much attention, and only a few examples are available.[3a, 3c] Here we report a manganese complex $[Mn(PN_3P)(CO)_2]Br$ containing a pincer backbone, as an efficient catalyst for formic acid dehydrogenation (Scheme 1).

Under the optimized condition, the complex afforded a TON of 15,200. To the best of our knowledge, this is considered one of the best TON achieved using a manganese-based complex with excellent selectivity. Mechanistic studies suggested that the imine arm participates in the formic acid activation/deprotonation step, emphasizing the importance of metal-ligand cooperativity during substrate activation to promote catalytic efficacy.

Detailed synthetic procedure, catalytic aptitude, kinetic experiments and mechanistic interpretation will be discussed.

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Materials -- Functional Nano-Materials and Nanotechnology

Stimuli Responsive Nano-agents: From Drug Delivery to Upstream Oil and Gas Applications

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Abstract:

Several concepts that have been successfully used for targeted drug delivery for medical diagnostics and treatment can lend themselves to some key oil and gas applications, despite the clear differences in the systems and environments involved. An example of such concepts is the utilization of stimuli responsive materials to deliver treatment or image contrast agents to specific targets in the human body, or the oil reservoir, without the side effects and unnecessary costs associated with excess release or delivery of agents to where they are not needed.

In-house program was initiated to develop nano-agents that can travel deep into the reservoir to collect reservoir information or deliver chemical treatments to hard-to-reach regions, autonomously by exploiting the induced or natural chemical and physical conditions in the reservoir. These regions are hardly accessed by conventional water or gas flooding techniques.

In this talk, a proof-of-concept on the effect of salt and surfactant gradients on the migration of reservoir nano-agents will be presented. The experiments use novel microfluidic devices and direct microscopic visualization to quantify the migration of solid colloidal particles (<1µm) under different gradients and to understand the underpinning electrokinetic and interfacial phenomena. The results demonstrate the ability of salinity and surfactant gradients to transport reservoir nano-agents up or down the imposed gradients in a predictable way. In this way, natural or induced gradients in the reservoir can be exploited to direct the reservoir nano-agents to certain regions in the reservoir for either recognizing or mobilizing the trapped resources.

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Materials -- Functional Material Synthesis and Characterization

A black absorber from Cu(I)-based complexes

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Since the major update of solar cells applications, “a black absorber” was synthesized to form glassy black single crystals capable of absorbing the solar radiation through the entire visible region and most of near-infrared (NIR) portion. This novel mixed-ligand Cu(I) coordination polymer has formed from colorless solution of Cu(I) precursor reacting with pyrazolate and azopyridine ligands. The single crystal X-ray diffraction analysis shows an extended infinite conjugation of the chromophoric units due to the “back-to-back” bridging ligands. The presentation exhibits the crystal structure and the spectral properties. In addition, the effect of varying the ligand substituents, on the molecular and crystal structures of the resulting products will be presented for further studies.

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Other Materials -- Functional Material Synthesis and Characterization

Smart Organic Crystals

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Elastic materials that are capable of stimuli-induced mechanical reconfiguration are indispensable for fabrication of mechanically tunable elements for actuation, including flexible electronics, artificial muscles, and microfluidics parts. The advanced materials that will qualify for these applications in the future must fulfill an extended list of requirements including reversible, rapid and controllable response that is proportional to the applied stimulus, and fatigueless operation over prolonged periods of time. Despite that elasticity is counterintuitive for crystals, there is an increasing number of reports of serendipitous observations of molecular single crystals that can hop, leap, bend, curl, crawl, expand, contract, twist, spin, explode, split, roll, or respond otherwise to external stimuli akin to soft, mesophasic materials. These dynamic crystals provide extreme and visually impressive demonstrations of the mechanical strain that can accumulate in the interior of molecular crystals and be released as mechanical energy. Mechanically reconfigurable molecular crystals—ordered materials that can adapt to variable operating and environmental conditions by deformation, whereby they attain motility or perform work—are quickly shaping up a new research direction in materials science, crystal adaptronics. Properties such as elasticity, superelasticity and ferroelasticity that are normally related to inorganic materials, and phenomena such as shape-memory and self-healing effects which are well established for soft materials, are now being reported for molecular crystals, yet their mechanism, quantification, and relation to the crystal structure are not immediately intelligible to the wider materials science research community. At the current stage of the understanding of their mechanical properties, the type of mechanical response from these materials remains hardly predictable, although it almost always is a result of the interplay between disintegrative and restorative factors.

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Sequence-controlled polymerization of Acrylamide monomers via RDRP technique

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Abstract Ref Number from the website: ID-6281
Session: Materials: Materials Synthesis

ABSTRACT

The ability to replicate the precision imposed by nature over monomer sequence, composition and structure is one of the key challenges facing polymer scientists. Natural polymers such as peptides, proteins, nucleotides and carbohydrates are precisely constructed, at the cellular level, according to their intended application and function. Synthetically, this level of precision is some way off, though progress over the last 30-40 years has significantly improved the limits of synthetic control now possible over the polymer primary sequence.

Herein, pure water has been utilized as the solvent for the preparation of multi-block copolymers of various acrylamide monomers at or below ambient temperature implying compatibility with biological systems and paving the way for the advanced polymers. An unprecedented level of control is imposed by the catalyst system which is prepared in situ via disproportionation of CuIBr/Me6TREN prior to introduction of monomer and initiator.

Nano-Co_3O_4 for Electrocatalytic Water for Oxidation

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Abstract Ref Number from the website: ID-5063
Session: Materials: Materials Synthesis

ABSTRACT

Nano-Co3O4 was used for electrocatalytic water oxidation due to its promising features for better performance and low cost. Enhanced electrochemical water oxidation performance of the nanoparticles can be achieved by mixing them with other types of highly conductive nano/micro-structured materials. Conductive polymers would be one of the candidates to achieve this goal. Here, we report our recently developed nano-Co3O4 and polypyrrole composites for enhanced electrochemical water oxidation. We chose polypyrrole as a support of nano-Co3O4 to obtain high active sites of nano-Co3O4 with high conductivity. Morphological and chemical characterization of the prepared materials were performed using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and X-ray photoelectron spectroscopy (XPS). After immobilizing them individually on fluorine doped tin oxide (FTO) substrate, their electrocatalytic properties toward water oxidation were investigated. The optimum composite materials showed significantly higher electrocatalytic properties compared to that of pure nano-Co3O4 and polypyrrole. Impedance studies indicated that the composite materials possess significantly less electron transfer resistance toward water oxidation reaction compared to that of only polypyrrole or nano-Co3O4. Due to the synergetic effect, the optimum nano-Co3O4 and polypyrrole composites could be represented as a novel and promising material for water oxidation.

Copper-based Hydrogels with Dicarboxylate Spacer Ligands for Selective Carbon Dioxide Separation

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Session: Materials: **Materials Synthesis**

ABSTRACT

Increasing levels of CO_2 emissions have attracted global research concern due to their fatal effects on the climate and environment. One technique that could limit CO_2 emissions from human activities into the atmosphere is Carbon dioxide Capture and Storage (CCS). It involves collecting, at its source, the CO_2 that is produced by power plants or industrial facilities and storing it away for a long time in underground layers, in the oceans, or in other materials. Hydrogels formed via coordination of polymeric ligands with metal ions show unique mechanical properties. They are specifically characterized by a reversible and dynamic metal–ligand coordination bond making them suitable for several applications most importantly gas separation and stimuli responsive material.In this presentation, we report a simple method for synthesizing copper-containing polymer hydrogels made from nontoxic poly(methyl vinyl ether-alt-maleic anhydride) (PVM-MA) in the absence or presence of added carboxylate ligands: dicarboxylates, such as adipate and terephthalate or tricarboxylates, such as nitrilotriacetate (NTA) and trisodium citrate. Our copper hydrogels are wet precursors to a new family of amorphous porous materials, consisting of a metal-polycarboxylate backbone and carboxylate spacer ligands between polymer strands engineered via non-covalent interactions.Upon addition of supplementary dicarboxylate ligands, rheological measurements revealed that the mechanical stability of the hydrogels was enhanced with the optimal ratio of polymer to dicarboxylate to Cu2+ was 10:4:2.5. This results aligns with scanning electron microscope (SEM) and cryo-SEM imaging and physical adsorption measurements which revealed the formation of pores. The Brunauer–Emmett–Teller (BET) surface area of the dried hydrogels was tunable with the addition of supplementary dicarboxylate ligands. Moreover, addition of dicarboxylate ligands increased the gas adsorption capacity and CO2 selectivity. However, the addition of nitrilotriacetate (NTA) and trisodium citrate resulted in decrease of crosslinking and deteriorated rheological properties which emphasizes that the hydrogel is suitable for stimuli responsive and sensing applications.Our copper-based hydrogel with dicarboxylate spacer ligands offers the possibility of a new material for post-combustion CO_2.

Development of Affordable localized-engineered cementitious composites for Building and Construction (AL-ECC)

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Session: Materials: Materials Synthesis

ABSTRACT

The material ingredients of engineered cementitious composite (ECC) or bendable concrete are similar to that of fiber-reinforced concrete, including cement, sand, water, few chemical additives and fibers but with significantly lower volume of the latter ingredient. AL-ECC constitutes an equally ductile to ECC cementitious composite by using 100% localized ingredients. It has been designed based on the existing technology of Polyvinyl alcohol-reinforced ECC (PVOH-ECC) for high tensile ductility (>3%) and tiny crack width (usually below 100 μm). AL-ECC retains the durability as PVOH-ECC (ability to withstand wear or damage), shows similar elastic pre-cracking and also has the ability of autogenous healing due to the intrinsically small crack width. The ability to undergo plastic deformation and not inelastic deformation as the typical concrete is attributed to the randomly distributed fibers. In AL-ECC structure, PV-OH fibers have been replaced with domestically available polyolefin fibers. This paper describes the strategic approach by replacing silica sand with other alternatives of sand-based materials as well as flying ash by other type of ash which correspond the highest volume cementitious materials on existed ECC technology. A-ECC also will enhance the ductility performance and reduce the cost by 40% compare to the existing technology of PVA-ECC which lead to further deployment of ECC in Building and Construction sector.

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR CATALYSIS SESSION

Development of Bismuth (oxy)sulfide Based Materials for Photocatalytic Applications.

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Session: Catalysis - Photo-Catalysis

ABSTRACT

NaLa1-xBixS2 solid solutions with tunable bandgaps were synthesized, and their optoelectronic structures and photocatalytic performance were investigated via experimental and theoretical approaches. The solid-solution powders with various La/Bi ratios were synthesized with Na2CO3, La2O3 and Bi2O3 as precursors and via sulfurization with flowing CS2 at 800 °C for 2 h. The Vegard's law behavior of cell parameters showed a perfect Bi/La solid solution in the cubic NaLa1-xBixS2 with the associated linear variation of the cell parameters. On the contrary, the combination of diffuse reflec-tance UV−Vis spectroscopy with density functional theory (DFT) calculations employing the HSE06 functional reveals a monotonic but non-linear variation of the bandgap of the solid solution. While consistent valence band maximum (VBM) was obtained in NaLa1-xBixS2—consisting mainly of S 3p orbitals—the conduction band minimum (CBM) was contributed by discrete Bi orbitals present at more positive potential than La. As a result, the slight inclusion of Bi caused a drastic shift in the bandgap, and 24% Bi substitution provided an absorption edge closer to that of pure NaBiS2. Systematic DFT calculations on NaLa1-xBixS2 determined the optoelectronic properties for improved photovoltaic and photocatalytic per-formance with a Bi-rich sample rather than a La-rich counterpart; i.e., there were larger absorption coefficients, smaller effective masses, and larger dielectric constants for Bi-rich samples versus La-rich samples. The NaLa1-xBixS2 particles dec-orated with Pt nanoparticles show maximum hydrogen evolution performance with x = 0.02-0.06 of Bi samples consistent with the compensating effects between photon absorption capacity and loss of electromotive force with decreasing bandgap.

Enhancement of Tetralin Hydrogenation over Supported Nickel Catalysts.

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Session: **Catalysis - Catalysts-Based Nanotechnology**

ABSTRACT

Hydrogenation and reduction of poly-aromatic compounds to enhance diesel and Jet fuels has received considerable attention recently to comply with global fuel specification and overcome future limitations. The characteristic properties of the current transportation fuels show high content of poly-aromatic compounds (mostly di-aromatic compounds) which reduces the fuel efficiency. In the literature, naphthalene and tetralin have been selected as a representative models for poly-aromatic compounds. The hydrogenation of naphthalene was studied intensively in the literature. However, less attention has been paid to its hydrogenated product (i.e tetralin (1,2,3,4-tetrahydronaphthalene)). It has been reported that hydrogenating tetralin is much more difficult than naphthalene. In this project an investigation was carried out to study the feasibility of using nickel catalytic systems synthesized by different methodologies and metal precursors for the hydrogenation of tetralin. The study entailed characterizing the synthesized catalyst using BET, AAS, TGA/MS, and XRD before and after the reaction. The catalytic activities of the synthesized catalysts were determined using a continuous down flow fixed bed reactor under different reaction conditions. The catalytic activity test results revealed that the performance of the synthesized in-house catalyst exceeded the activity achieved by literature nickel catalysts at lower reaction conditions. Different activities were recorded for different reaction parameters. A notable difference was observed in the trans/cis ratio of the products using catalysts prepared with different nickel precursors. The spent catalysts were post-characterized and showed significant amount of carbon laydown.

Novel Bifunctional, Trimetallic CuxZnyVO4 Microarchectures for Solar-Driven Water Splitting and Waste Water Remediation.

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Session: Catalysis - Photo-Catalysis

ABSTRACT

Innovative solar-driven conversion strategies are required to effectively consume the available resources for non-traditional energy harvesting and waste product conversions, to ensure environmental sustainability. In this article, we reported the photoelectrochemical (PEC) properties of trimetallic CuxZnyVO4 (Innovative solar-driven conversion strategies are required to effectively consume the available resources for non-traditional energy harvesting and waste product conversions, to ensure environmental sustainability. In this article, we reported the photoelectrochemical (PEC) properties of trimetallic CuxZnyVO4 (CZV) heterostructures prepared by wet chemistry technique. To facilitate the process, we further added Na2S as a sacrificial agent to the electrolytic solution. Elemental analyses via XPS and EDX confirm the existence of Cu, Zn and V at the ratios 1;2 and 3. The deficient oxygen, surface defects and cathodic characteristics of Cu, efficiently facilitate the charge transfer and lowered the charge recombination. Trimetallic CuxZnyVO4 heterostructure photocathode with Na2S produced significant photocurrent density, 3 times greater than the sample without Na2S. Appropriate surface modification demonstrated an onset potential for cathodic photocurrent as high as 0.51 VRHE, a 5.2 mA cm-2 of photocurrent at 0 VRHE and a half-cell solar-to-hydrogen conversion efficiency of 1.1% at 0.37 VRHE. The potential of CZV photocatalyst was investigated by degrading Congo Red (CR) and Crystal Violet (CV) dyes using a UV–visible spectrophotometer. These CZV showed enhanced dye removal (100%) due to reduced bandgap 2.68eV and high surface area (84 m2/g). The present study provides new insights into techniques for the preparation of particulate CZV microarchitectures environmental friendly solar-driven remedies.) heterostructures prepared by wet chemistry technique. To facilitate the process, we further added Na2S as a sacrificial agent to the electrolytic solution. Elemental analyses via XPS and EDX confirm the existence of Cu, Zn and V at the ratios 1;2 and 3. The deficient oxygen, surface defects and cathodic characteristics of Cu, efficiently facilitate the charge transfer and lowered the charge recombination. Trimetallic CuxZnyVO4 heterostructure photocathode with Na2S produced significant photocurrent density, 3 times greater than the sample without Na2S. Appropriate surface modification demonstrated an onset potential for cathodic

photocurrent as high as 0.51 VRHE, a 5.2 mA cm-2 of photocurrent at 0 VRHE and a half-cell solar-to-hydrogen conversion efficiency of 1.1% at 0.37 V RHE. The potential of CZV photocatalyst was investigated by degrading Congo Red (CR) and Crystal Violet (CV) dyes using a UV–visible spectrophotometer. These CZV showed enhanced dye removal (100%) due to reduced bandgap 2.68eV and high surface area (84 m2/g). The present study provides new insights into techniques for the preparation of particulate CZV microarchitectures environmental friendly solar-driven remedies.

Photocatalytic Oxidation of Organic Substrates by Ru/Cu Hetero-metallic Complexes with Dioxygen as the Unique Oxygen Atom Source.

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Abstract Ref Number from the website: **ID- 4334**
Session: **Catalysis - Photo-Catalysis**

ABSTRACT

Currently, processes using atmospheric dioxygen in fine chemistry for oxidation reactions are limited mainly due to the difficulty to activate such a stable molecule. However, some Fe(II) and Cu(I)- enzymes i.e. oxygenase are capable to realize this activation yielding to oxidizing species. After a two electron oxidation of a substrate, Cu(I) and Fe(II) are recovered and their subsequent reduction are then required to regenerate the reduced active species.

With the aim to develop new “eco-aware” catalysts we designed an original heterobinuclerar Ru-Cu complex constituted by the covalent association of a Ru-based photosensitizer and a Cu-based catalyst. Irradiation at the appropriate wavelength, in the presence of a sacrificial electron-donnor (D), results in the reduction of the Cu(II) system into Cu(I) thanks to electron transfers (E.T) from the electron-donnor to the copper subunit via the excited photosensitizer. Photocatalytic experiments showed that the synthesized complex was able to selectively oxidize sulfides into sulfoxides using O2 as the unique oxygen-atom source. In order to perform oxygenation reactions, the use of dioxygen as an oxygen atom source appears to be an ideal solution.

Reference: Iali. W, et al Angew. Chem. Int. Ed. 2015, 54, 8415

Nanocatalysts for a circular carbon economy.

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Abstract Ref Number from the website: **ID- 4368**
Session: **Catalysis - Catalysts-Based Nanotechnology**

ABSTRACT

The natural carbon cycle needs large scale CO2 conversion to accommodate the excess emissions. A sustainable circular carbon economy would require new pathways since the current technologies and CO2 market are far too insufficient. For a sizeable CO2 fixation, we chose a redox path of dry reforming and a favorable, non-redox reaction of CO2 cycloaddition to epoxides to provide more than 10 gigatons of CO2 fixation, a 2050 target set by the National Academy of Sciences of the USA. In dry reforming of methane, we developed a Ni-Mo-MgO nanocatalyst that runs over 850 hours of continuous activity, a record for non-noble catalysts without coking or sintering. We identified a novel mechanism that requires nanocatalysts to be on single crystal edges (NOSCE). For the non-redox CO2 fixation into cyclic carbonates, we developed a new imidazolinium catalyst forming a Lewis acid/base pair that catalyzes even ambient pressure CO2 without any need for solvents, co-catalysts or metals.

Hydrogen Production from Liquid Hydrocarbon Fuels via Thermo-neutral Reforming (TNR) with Multi-Component Catalyst.

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Abstract Ref Number from the website: **ID- 5062**
Session: **Catalysis - Catalysts-Based Nanotechnology**

ABSTRACT

Hydrogen demand in the refining sector is expected to continue its growth driven mainly by stricter fuel specifications. In addition, hydrogen-based fuel cells for automotive and stationary applications are gaining popularity for various reasons including their higher efficiencies and lower emissions. The infrastructure to deliver hydrogen is currently inadequate and the storage of hydrogen on-board a vehicle remains a major technical and economic hurdle. Use of liquid hydrocarbon fuels to generate hydrogen is being considered as an immediate solution for large scale hydrogen production. For this purpose Ni-based alumina supported multi-components catalysts are prepared by sequential impregnations of metals using wetness incipient method. Novel catalyst preparation techniques were employed to produce active and stable reforming catalysts for liquid hydrocarbons reforming to suppress catalyst deactivation. For mobile applications, liquid fossil fuels like diesel are suitable due to their high energy density, their easy storage and their already existing distribution infrastructure. However, diesel reforming is known as a major challenge due to its high carbon content, aromatics, and sulfur, which play a major role in catalyst deactivation. In this study, a new fuel delivery technique (atomization) was investigated for diesel reforming. An ultrasonic injector was used to mix all feedstock (fuel, air and steam) before it reaches the catalyst bed. The new method has improved the thermo neutral reforming (TNR) catalyst performance and stability with diesel. Monolith-based TNR catalysts of various sizes were prepared and their performance was evaluate in a fixed bed reactor with heavy naphtha and diesel as feedstocks. Compared to any other catalyst structure such as pellets or extrudates, a significantly lower pressure drop is observed when monolithic catalysts are used. The newly developed TNR catalyst showed stable performance with heavy naphtha as well as diesel for hydrogen production.

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2020)

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Characterization of the Synthesized Zeolite-Y Catalysts by XRD Data and Rietveld Method

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Abstract Ref Number from the website: **ID- 4480**

Session: **Catalysis - Catalysts-Based Nanotechnology**

ABSTRACT

This paper describes the synthesis, purity, crystallinity and Si/Al molar of the in-house zeolite-y catalysts by XRD data and Rietveld method. The zeolite-Y with high crystallinity and yield was synthesized. The zeolite exhibited better performance in crude oil directly hydrocracking to produce high-quality feedstocks for steam cracking or catalytic reforming [Ding, Sitepu, Bogami et al., (2021). ACS Omega, **6**, 28654−28662). The purity and crystallinity percentage of the synthesized zeolite-Y catalysts have been characterized by X-ray powder diffraction (XRD) data. In the present study, Rietveld refinement with the generalized spherical harmonic description for correction of the preferred orientation in powder diffraction analysis for both crystal structure refinement and quantitative phase analysis [Sitepu et al. (2005). *J. Appl. Cryst.* **38**, 158-167; Sitepu (2009). *Powder Diffr*. **24**, 315-326] has been extended to describe crystal structure and texture in all the XRD data sets of the synthesized zeolite-Y powders. The results revealed that the structural refinement parameters obtained from the Rietveld refinement with the generalized spherical harmonic description, agreed well with the corresponding single crystal structure. In addition the generalized spherical harmonic description provides better results for the materials investigated in the present study than that of the March model. Therefore the generalized spherical harmonic approach should be used for preferred orientation correction in XRD Rietveld analysis, for both crystal structure refinement and phase composition analyses zeolite–Y catalysts.

Au9 –Nanoclusters Photocatalysis Deposited on Titania Surfaces

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Abstract Ref Number from the website: ID- 5644
Session: Catalysis - Photo-Catalysis

ABSTRACT

In this work, chemically made clusters stabilised by organic ligands, Au9 (PPh3)8(NO3)3 (Abbreviated Au9), deposited on titania surfaces are investigated by using various surface sciences techniques to study gold clusters and the effects of titania surfaces. Supported size specific metallic nano-clusters have emerged as superior catalysts in a few cases such as water splitting process for hydrogen production and CO oxidation process but until now fabrication and activation of catalysts using chemically synthesised atomically precise gold (Au) clusters supported on titania has not been well understood. Chemical reactivity of metal clusters is determined by three main factors: (a) size of clusters, (b) geometric arrangement of atoms forming clusters and (c) electronic structure. Also, metal oxide supports play an important role in changing the catalytic activity of nanoclusters. In this study, various surface techniques were used to investigate the above factors using various substrates and various pre-treatment methods. Chemical compositions of clusters deposited on titania surface and removal of ligands after heat treatment were monitored using XPS. The heating process caused the Au clusters to partially agglomerate with the remaining isolated precise Au clusters. Aberration corrected HAADF-STEM with low electron-beam acceleration voltage was used to resolve the detailed structure of ultra small protected Au9 clusters deposited on titania nanosheet at atomic resolution for the first time. Such microscopes are capable of directly determining the geometric structure of Au9 clusters deposited on substrates. We compared experimental Au9 structures using STEM with DFT calculations of clusters of nine Au atoms in the gas phase. While substrate influence on Au9 structure is missing in DFT calculations, it is possible to classify structures of Au9 clusters deposited on titania as found experimentally using STEM. AFM and STM observations show nanoclusters are highly distributed and their average size was measured. STM showed an individual Au9 deposited on titania nanosheet. In addition, Metastable Induced Electron Spectroscopy (MIES) was applied to quantitatively determine valance electronic structure of supported Au clusters. The results of this study are very important to the surface science community and outcomes are potentially useful in improving understanding of key factors affecting catalytic activity of atomically precise support immobilised clusters

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Development of Bismuth (oxy)sulfide Based Materials for Photocatalytic Applications

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Abstract Ref Number: ID-3872
Session: Catalysis

ABSTRACT

NaLa1-xBixS2 solid solutions with tunable bandgaps were synthesized, and their optoelectronic structures and photocatalytic performance were investigated via experimental and theoretical approaches. The solid-solution powders with various La/Bi ratios were synthesized with Na2CO3, La2O3 and Bi2O3 as precursors and via sulfurization with flowing CS2 at 800 °C for 2 h. The Vegard's law behavior of cell parameters showed a perfect Bi/La solid solution in the cubic NaLa1-xBixS2 with the associated linear variation of the cell parameters. On the contrary, the combination of diffuse reflec-tance UV−Vis spectroscopy with density functional theory (DFT) calculations employing the HSE06 functional reveals a monotonic but non-linear variation of the bandgap of the solid solution. While consistent valence band maximum (VBM) was obtained in NaLa1-xBixS2—consisting mainly of S 3p orbitals—the conduction band minimum (CBM) was contributed by discrete Bi orbitals present at more positive potential than La. As a result, the slight inclusion of Bi caused a drastic shift in the bandgap, and 24% Bi substitution provided an absorption edge closer to that of pure NaBiS2. Systematic DFT calculations on NaLa1-xBixS2 determined the optoelectronic properties for improved photovoltaic and photocatalytic per-formance with a Bi-rich sample rather than a La-rich counterpart; i.e., there were larger absorption coefficients, smaller effective masses, and larger dielectric constants for Bi-rich samples versus La-rich samples. The NaLa1-xBixS2 particles dec-orated with Pt nanoparticles show maximum hydrogen evolution performance with x = 0.02-0.06 of Bi samples consistent with the compensating effects between photon absorption capacity and loss of electromotive force with decreasing bandgap.

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Highly Efficient Ruthenium-Catalyzed Reductive N-Formylation of Amines: Utilization of CO2 as C1 Building Block

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Abstract Ref Number: ID-6401
Session: Catalysis

ABSTRACT

Production of bulk and value-added chemicals using abundant and inexpensive CO2 as C1 building block has the potential to become an essential part of the sustainable chemical industry.1 However, the thermodynamic stability and kinetic inertness of CO2 pose a significant challenge for such a methodological development.2 The design of catalytic systems to overcome these issues is thus of principal research interest. CO2 can be utilized in Nformylation of amines, where it acts as carbonyl source in N-formylation of amines.3 Formamides are considered as important intermediate in synthesis of value-added chemicals, namely, pharmaceutical materials, N-heterocycle, oxazolidinones and cancer agents.4 Formyl groups are also used in preparation of amino acids and formamidines. Herein, we report a ruthenium-pincer-type complex as a highly efficient catalyst towards N-formylation of amines with CO2 and H2 (Scheme 1). A variety of amines are converted to their corresponding formamides with excellent reactivity and selectivity. Even in a single batch operation at low catalyst loading, high TON have been achieved for N-formylation.

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The Gulf International Hotel, Kingdom of Bahrain
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Effect of Zeolite Y modification on Reaction Performance of Crude Oil Hydrocracking

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Abstract Ref Number: ID-4053
Session: Catalysis

ABSTRACT

Hydrocracking is one of the most important heavy oil conversion processes in modern refineries and petrochemicals plants. Hydrocracking is mainly used for VGO conversion. Few studies were conducted for direct crude oil conversion. In this presentation, the effect of hydrocracking catalysts, playing critical role in determining the product slates and properties, on crude conversion is studied. Zeolite Y is a widely used cracking component of the commercialized hydrocracking catalysts. Its pore structure and acidity can be modified by various chemical or steaming treatments, and have critical effect on the catalyst reaction performances. Zeolite Y was modified by different methods to generate modified zeolites with varied silica-to-alumina ratios, mesoporosity, and acidity. The catalysts were characterized with XRD, BET, NH3-TPD, XRF, 27Al and 28Si solid NMR. The reaction performances were evaluated in pilot plant. The results show that to achieve the optimum performance in heavy oil conversion, the pore structure and acidity of the catalysts need to be well balanced. Combining the optimal operating conditions with the modified Y zeolite, the 540°C+ residue fraction can be completely converted.

Speciation analysis of Chromium in catalyst samples

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Abstract Ref Number: ID-5017
Session: Catalysis

ABSTRACT

Hydrocracking is one of the most important heavy oil conversion processes in modern refineries and petrochemicals plants. Hydrocracking is mainly used for VGO conversion. Few studies were conducted for direct crude oil conversion. In this presentation, the effect of hydrocracking catalysts, playing critical role in determining the product slates and properties, on crude conversion is studied. Zeolite Y is a widely used cracking component of the commercialized hydrocracking catalysts. Its pore structure and acidity can be modified by various chemical or steaming treatments, and have critical effect on the catalyst reaction performances. Zeolite Y was modified by different methods to generate modified zeolites with varied silica-to-alumina ratios, mesoporosity, and acidity. The catalysts were characterized with XRD, BET, NH3-TPD, XRF, 27Al and 28Si solid NMR. The reaction performances were evaluated in pilot plant. The results show that to achieve the optimum performance in heavy oil conversion, the pore structure and acidity of the catalysts need to be well balanced. Combining the optimal operating conditions with the modified Y zeolite, the 540°C+ residue fraction can be completely converted.

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR MATERIALS CHARACTERIZATION SESSION

The impact of the deposition pressure in depositing cadmium telluride thin films on ultra-thin glass substrate via Close Spaced Sublimation (CSS)

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Abstract Ref Number from the website: ID-6301
Session: Oral, Materials: Material Characterisation

ABSTRACT
CdTe thin films were grown under the pressure range of 1 Torr to 200 Torr to explore the impact of deposition pressure on CdTe thin-film properties. The microstructural, compositional and optoelectrical characteristics were examined. X-ray Diffraction (XRD) analysis revealed the cubic phase crystallite CdTe films with (111) preferential orientation. Scanning Electron Microscopy (SEM) demonstrated that the CdTe morphology and grain size could be regulated via the deposition pressure, whereby maximum grain growth was detected at low pressure (1 - 5 Torr). The thickness of CdTe films was reduced from 6 µm to 1.5 µm with the rise in deposition pressure. Moreover, the optical direct energy gap was derived in the range of 1.65 - 1.69 eV for the pressure value of 200 Torr to 1 Torr. Carrier density and resistivity were found to be in the order of 1013 cm-3 and 104 Ω cm, respectively. The experimental results suggest that the pressure range of 1 - 5 Torr may be ideal for CSS-grown CdTe films on flexible ultra-thin glass (UTG) substrates. Keywords: cadmium telluride; thin film; close spaced sublimation; deposition pressure; ultra-thin glass.

Acknowledgments
The authors acknowledge the National Plan for Science, Technology, and Innovation (MAARIFAH), King Abdulaziz City for Science and Technology, Kingdom of Saudi Arabia for its grant with award No. 13-ENE2229-02. parameters WOB and RPM by a small percentage (0-5%), in a Constrained Random Search (CRS) way.

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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Microbial and Phase Compositional Determination of Deposits from Refineries to Investigate the Root Causes Failure Analysis

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Abstract Ref Number from the website: ID-6403

Session: Oral, Materials: Material Characterisation

ABSTRACT

This paper described the microbial and chemical compositional analyses of the deposits from the refinery plants. This specific plant contains high level of H2S, and therefore, if it leaks will expose refinery and community personnel to unnecessary health risks. Additionally, the repetitive re-boiler and piping leaks experienced in this crucial plant are likely caused by microbial activities as well as various chemical reactions occurred in this high H2S system. These chemicals can also cause preliminary failures and slowdown the productions. To support the investigation team from the plants, the authors conducted the lab-based study to identify the root causes of failures, and quantitative phase composition of deposits from the affected failure equipment by using the quantitative polymerase chain reaction and Rietveld refinement of X-ray powder diffraction (XRD) data.

The results revealed that low number of general bacteria and corrosive SRB (101-103 cells/g) was detected in the solid samples collected from the 2nd and 4th baffle, and the ceiling of the outer shell, whereas the samples collected from the 3rd baffle and the bottom of the outer shell showed the below detection limit of microbes obtained from quantitative polymerase chain reaction. Additionally, the quantitative phase analysis of XRD data of the deposits obtained from Rietveld refinement revealed that the deposits mainly consist of iron sulfides corrosion product in the form of mackinawite [FeS], greigite [Fe3S4] and pyrite [FeS2] and iron oxide corrosion product in the form of magnetite [Fe3O4] and goethite [FeOOH] with the additional sulfur phase. The findings are supported by the presence of corrosive SRB, diverse iron sulfides species with possible biological origin, and sulfur suggesting that the feasibility of biocide treatment on feed crude in refinery plants needs to be investigated with a great care.

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Advanced X-ray analytical techniques to support the development of innovative materials

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Abstract Ref Number from the website: **ID-4450**

Session: **Oral,** **Materials:** **Material Characterisation**

ABSTRACT

Determination of Iron corrosion products Iron corrosion products such as " FeS, FeS4, Fe3O4" behave differently under the microscope. In this project using advanced X-ray analytical techniques to support the development of innovative materials, the differences between those types and how they actually look like under the microscope has been showed.

Challenges And Improvements For An Accurate Mercury Analysis In The Oil And Gas Industry

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Abstract Ref Number from the website: ID-6405
Session: Oral, Materials: Material Characterization

ABSTRACT

Mercury is an undesirable contaminant in the oil and gas industry due to its effect in aluminum embrittlement and catalyst poisoning downstream. [1] Its concentration in both sweet gas and other hydrocarbons (crude oil, NGL, condensates, etc) is critical for the integrity of the processes. [2,3] Environmentally, mercury needs to be monitored to prevent pollution of the aquatic ecosystem, such fish and other microorganisms. The strange behavior of mercury compounds therefore calls for special treatment of different samples, which therefore makes its accurate measurement a challenge. This study will describe different ways that can be implemented to accurately quantify mercury and close the mass balance in all forms of mercury in the oil industry.

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PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR CARBON MANAGEMENT SESSION

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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The insignificant role of dry reforming of methane in the CO2 emission relief

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Abstract Ref Number from the website: ID- 5707 Session: Carbon Capture and its Applications

ABSTRACT

CO2 utilization (CDU) or reduction of at least 30 gigatons of CO2 (GtCO2)/yr is needed to meet the Paris Agreement objectives to keep global warming below 2 °C. A meaningful impact can only be achieved when CDU is conducted for profitable industrial applications in addition to net-zero CO2 emissions.1-3 In this context, dry reforming of methane (DRM) has been proposed and marketed as a potential solution that may achieve decarbonization at the scale of multi-GtCO2/yr. 4 In DRM, methane (CH4) and CO2 react in a 1:1 ratio to afford a mixture of CO and H2, known as syngas ($CO_2 + CH_4 \rightarrow 2CO + 2H_2$). This syngas was considered as a suitable feed for the direct synthesis of dimethyl ether (DME), an alternative transportation fuel for diesel engines. With low capital investments, this direct process is envisaged as an efficient approach for DME synthesis over an indirect pathway through methanol dehydration.5 Unfortunately, claiming DRM to fuels to meet the goal of CO2 emission relief is likely misleading and inappropriate, based on the data acquired from various industrial reforming processes.

While DRM may appear like a simpler process than steam methane reforming (SMR), as it does not require the use of steam, its energy demand is higher due to the chemically inert nature of CO2. Hence, DRM is operated at high temperatures and needs at least 340 kJ/molCH4, resulting in 0.38 CO2e/molCH4 (1 GJ = 50.5 kg CO2 equivalent as per U.S. EIA). 6 Thus, DRM consumes 1.38 moles of CH4 for the utilization of 0.62 moles of CO2 in the best-case scenario. Furthermore, for each mole of CO2/molCH4 utilized in the primary reforming process, it re-emits 0.67 moles of CO2/molCH4 during the production of DME ($3\,CO + 3\,H_2 \rightarrow DME + CO_2$). 7 Therefore, considering the energy-intensive nature and low CDU potential of the DRM to DME pathway, the overall transformation of natural gas to the final products will be analogous to those of the modern CH4 reforming technologies.8 Figure 1. Well to wheel efficiencies of CNGV and DRM-DME vehicle.

Importantly, well to wheel (WTW) efficiency and CO2 emissions of a DME-DRM based vehicle are approximately the same as those of compressed natural gas vehicle (CNGV), in addition to the conceivable higher capital and operating investments (see Figure 1). Although the exploitation of renewable energy has also been proposed to make DRM CO2 neutral,9 such energy can be more efficiently utilized by fuel cell electric vehicles

(FCEV) and battery electric vehicles (BEV) with zero tailpipe 2 emissions.10 In summary, even when the energy penalty in this endothermic process is not considered, DRM will, at its best, make negligible contributions to the CO2 emission relief. Since CH4 is the primary energy source and CO2 only serves as a carrier, fuels from DRM will create the same amount of net CO2 emission per energy unit, similar to CH4 combustion and SMR.11 Broad deployment of DRM for such a purpose will be a costly distraction. DRM might serve the business need for value-added manufacturing, but the goal of CO2 emission relief has to be realized with low-carbon energy.12

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THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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Ammonia Decomposition and Hydrogen Separation Using Membrane Reactors

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Abstract Ref Number from the website: ID- 5004 Session: Carbon Capture and its Applications

ABSTRACT

Hydrogen is the primary fuel source for fuel cells. However, its low volume density, and storage and transport difficulties are major obstacles for its practical utilization. Ammonia is a promising hydrogen carrier because of its high hydrogen density and ease of liquefaction and transportation. Ammonia cracks catalytically into nitrogen and hydrogen, followed by separation using membranes. Currently, this two-step process produces high purity hydrogen. The operating temperature of an ammonia cracker and separation system are similar, suggesting the advantage of coupling both functionalities into a single membrane reactor to produce pure hydrogen in a simplified overall system. In this study, several ammonia cracking catalysts and hydrogen separation membranes have been combined and investigated.

Catalysts for ammonia decomposition have been developed using metal oxide-supported Ni- and Ni-Ru-based catalysts. Among the Ni catalysts investigated, the activity of Ni/Y2O3 was sufficiently high at around 600°C and showed stable activity for 1000 h at 700°C in an accelerated aging test. These catalysts were selected for use in a Pd membrane reactor for economic hydrogen production. Supported thin film palladium and palladium alloy membranes were prepared similarly to methods described in the literature for hydrogen separation from ammonia decomposition products. The membranes were tested with ammonia/H2/N2 gas mixtures at 450-550°C to demonstrate their chemical and thermal stability and its comparison with a packed-bed catalytic reactor. The membrane reactor test results and next steps will be presented.

Advanced Analyses of Amine Solutions in Support of Amine Gas Sweetening Process

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Abstract Ref Number from the website: ID- 6094 Session: Carbon Capture and its Applications

ABSTRACT

Stemming from the high demand on natural gas globally, maintaining integrity of natural gas production process is crucial. Due to the presence of acid gases within the stream, such as carbon dioxide, carbon sulfide, and carbonyl sulfide, many problems could arise including impacts on flow assurance, corrosion and healthiness of the system. Acid gas treatment processes by amine solvents, such as diglycol amine, that enable the removal of acid gases via adsorption/desorption reactions are used. These amine solvents are circulated after the sour gases' removal process; thus, the quality of the amine solvents must be monitored closely and checked against internal QA/QC to ensure efficient operations. Therefore, a detailed amine characterization, that consists of a package of eight major assessments, were developed. The assessments examine: I) basicity of the amine by measuring the pH at 25°C and specific gravity at 60°F as it is essential for flow and pipelines design calculations. II) amine strength which represents the amount of free amine available for acid pick-up. III) total amount of nitrogen to facilitate nitrogen balance calculations considering the nitrogen rich complex environment. IV) amount of ammonium ions in reflux water since its buildup may causes limitation in acid pick-up. V) elemental analysis to quantify metals to monitor corrosion, foaming, and facilitate calculation of bond amine. VI) quantitative phase of solid particulates to identify the root cause of the particulates and stop their generation VII) detailed compositions and contaminants to understand solvent quality. VIII) advanced characterization of additives based on amine formula used in treatment. This original and extensive study - performed in-house - establishes new knowledge, reduces the process upsets, saves a significant amount of money and resources, and ensures meeting gas treatment specifications and production continuity.

Preliminary Assessment on Carbon Capturing for Sustainability (CSS)

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Abstract Ref Number from the website: ID- 6199 Session: Carbon Capture and its Applications

ABSTRACT

Qualities analysis is governed to review current and future application models of Caron Sequestration Sustainability (CCS) and bioconversion addressing in low carbon emissions. A number of new promising CCS technologies are described and discussed with their future development prospects (e.g fuel cells, membranes, chemical looping) Specific case studies of organization involved in CCS have enabled comparisons to be drawn in relation to the financial cost and practicality of implementation. It has been noted that countries must provide incentives for organizations assisting to implement carbon capture. Investors must be met with sufficient favorable conditions to venture carbon capture technology. And governments may achieve this be legally restricting the allowed amount of carbon emissions from industry. Results of study show that oxyfuel, pre-combustion and post combustion are most prevalent technologies to implement in capturing carbon in chemical industries such Petra-Nova Plant Operation Texas.

Drawbacks and consequent benefits will be discussed with possible retrofitting to existing plants. The Implementations of CCS has been notably been observed cement industry, though there is much scope in refineries and other sectors excluding carbon for storage. The use of Carbon Capture technologies will aid in sufficient examining in retrofitting application and alter process principle schemes to have a more efficient and recycled regime of rich carbon dioxide gas product. Furthermore, Public awareness is an important aspect in ensuring that CCS projects are fulfilled. People should be well-informed of the threats caused by carbon emission, with their influence to be paramount importance in convincing governments industry of the necessity of adopting CCS technologies.

Acknowledgments: Thanks and appreciation to the advisor Dr Fatima Mahiedine at University of Bradford. Extended grateful Kuwait Institute for Scientific Research (KISR) for continued support and motivation in engagement for new engineers at PRC.

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR GREEN ENERGY SESSION

Hexagonal boron nitride/ graphene composite and its application as electrode material in asymmetric supercapacitor application

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Abstract Ref Number from the website: ID- 3863
Session: Materials: Green Energy

ABSTRACT

Owing to their high energy density and power density, supercapacitors reach great attention as high-performance energy sources for advanced technologies. Recently, 2D nanomaterials have widely investigated as effective electrodes in supercapacitors due to their unique properties especially the hybrids of two different materials with different charge storage mechanisms. Graphene and boron nitride composite can be regarded as the ideal material for supercapacitor application on account of the EDLC mechanism and pseudocapacitive nature of the hexagonal boron nitride. Relative rotation of layers causes different stacking angles between graphene and boron nitride in every percentage that can affect the bandgap. In some cases, small band gaps are generated and quantum confinement can be noticed. These differences lead to different behaviors in electrochemical performance.

In this work, the hydrothermal methods were used to prepare different percentages of h-BN/GO hybrids and Co3O4/h-BN/GO hybrids and different characterization techniques were applied to determine the structural, electrical, thermal properties of the composites. The thermal stability of h-BN/GO composites was studied by TGA and DSC and the results from all show that there is high thermal stability for all the hybrids. The specific surface areas were calculated by the conventional BET method which shows that with the increase in the amount of GO in h-BN/GO hybrids the surface area increases.

This work supports the synergistic effect of graphene and boron nitride in the asymmetric supercapacitor as a positive electrode and rGO as a negative electrode exhibited high specific capacitance of 132 F/g and high stability after 5000 cycles with a retention of 71%.

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Enhanced energy storage using cobalt-polyaniline hybrid assembly- Influence of electropolymerization protocols

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Session: Materials: Green Energy

ABSTRACT

Cobalt-polyaniline composites have been used in the electrode materials to improve the stability and dispersion of the electroactive sites, which is useful in various electrochemical applications, such as batteries, supercapacitors, sensors and solar cells. The synergistic effect of such composite materials was attributed to surface properties in which metal oxide particles were distributed evenly over the polymer matrices.

In the present study, the morphologies and the electrochemical properties of the composite electrode materials have been investigated toward energy storage applications. Two different electropolymerization protocols have been implemented to produce composite electrode materials, i.e. co-deposition and post deposition. Potentiodynamic technique has been used in various electrochemical cells in order to control particles distribution within the polymer matrices, and thus achieve the optimal conditions of current density and offset potential. The electrocatalytic properties were evaluated by using linear sweep voltammetry. The results show that using post deposition protocol to produce the cobalt-polyaniline composites has superior electrocatalytic properties over the composite materials produced from co-depositions protocol.

IGCC Soot Ash Recovery Unit In Jazan Complex

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Session: Materials: Green Energy

ABSTRACT

Soot Ash recovery process is technology applied for the first time in Saudi Aramco at Jazan Complex – Integrated Gasification Combined cycle (IGCC) Soot Ash recovery unit (SARU). Soot Ash recovery process is deployed in Jazan IGCC SARU to support the Gasification process in processing soot and by providing the filtrate water. The gasification process contains Burner, Gasifier and Syngas effluent cooler (SEC) system to convert high sulfur fuel oil (or vacuum residue) into synthesis gas produce and at a controlled "soot production rate". The soot / ash particles on vacuum residue (designed to be 0.5-1.0 wt.-%) shall be removed in Gasification system by using filtrate water recovered from SARU. From the gasification of vacuum residue, more than 95% of Soot /Ash is removed from the Syngas product as soot slurry with maximum 10 wt% soot. On the other hand, Soot ash recovery technology is deployed in Jazan IGCC SARU plant to enhance the recovery of metal oxides (Ash) as by-product and reduce emissions and protect the gasification system from possible erosion by those soot solid particles. In SARU, the production around 20 ton/day of Ash and above 16 ton/day of filtrate water as feed of Gasification system.

This presentation will give more details about the mechanism and benefits of deploying this technology in Jazan Refinery IGCC SARU.

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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Advancement Hydrogen Fuel Cell Technology

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Session: Materials: Green Energy

ABSTRACT

A hydrogen fuel cell generates energy by combining hydrogen and oxygen, making it a potential source of an electric power. The following paper presents the characteristics, operating theory, implementations, benefits, and drawbacks of the novel hydrogen fuel cell technologies available. It also covers the techniques for producing and storing hydrogen, which is the main fuel for a fuel cell. Additionally, a brief comparison of internal combustion vehicles (ICEV) and hydrogen fuel cell vehicles (FCV) is presented. The findings indicate that hydrogen fuel cell technologies have a general framework, a high-performance range of 40 to 60%, an optimal temperature range of 70 to 1000oC, and a reduced natural effect. At the end, a comparative study of five major power generating system is also performed.

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An Innovative Downhole Energy Harvesting System

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Abstract Ref Number from the website: ID- 5687
Session: Materials: Green Energy

ABSTRACT

1. Objectives/Scope: Downhole power harvesting is an enabling technology for a wide range of future production systems and applications including self-powered downhole monitoring, downhole robotics, and wireless intelligent completions. This paper presents the field experience of an innovative energy harvesting system that was successfully deployed and tested in the harsh downhole conditions of an oil producer.

2. Methods, Procedures, Process: There is a critical need for robust and reliable downhole power generation and storage technologies in order to push the boundaries of downhole sensing and control. This paper provides an analysis of available ambient energy sources in the downhole environment, and various energy harvesting techniques that can be employed to provide a reliable solution. Advantages and limitations of conventional technique like turbine are compared to advanced energy harvesting technologies. The power requirements and technical challenges related to different downhole applications have also been addressed. The field experiences of the novel flow based energy harvesting system are presented, including the details of both the lab and field prototype design, deployment and testing.

3. Results, Observations, Conclusions: The field experiences of a novel flow based downhole energy harvesting system are presented. The design and testing details of the lab prototype of the system are discussed. The retrofit system was successfully installed and tested at the depth of 5000 ft in an oil producer. The successful deployment and testing of the field prototype effectively harvested 10s of watts of continuous hydraulic power that was converted into usable electrical power with a downhole electrical generator. The lessons learned and the way forward are elaborated in length.

4. Novel/Additive Information: The first ever successful demonstration of an innovative downhole energy harvesting system is presented in this paper. The ground breaking technology has the potential to revolutionize the applications including self-powered downhole monitoring, downhole robotics, and wireless intelligent completions.

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The Potential and Challenges of Using Solar and Wind Energy for Oil and Gas Production Operations and Applications

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Abstract Ref Number from the website: **ID- 5691**
Session: Materials: **Green Energy**

ABSTRACT

The availability of reliable sufficient electrical power supply especially in remote off-grid oil fields is a critical obstacle that faces several of those fields' development projects, from deploying Electrical Submersible Pumps, to installing Multiphase Boosting Compressors, and several other applications. The Middle East is blessed with an abundant solar radiation and enormous open land which represents a great potential of harnessing solar and wind energy, adding them to the massive oil resources in the region. This paper reviews solar and wind energy technologies and compare them against other remote power drivers like electrical motors, diesel engine, and gas turbines. The economic and technical factors for the solar and wind solutions are considered, and a number of case studies with state of the art renewable energy technologies used for remote power supply are presented. The paper identifies, the potential and challenges of using these renewable energies for remote power supply in oil fields, as well as states a road map to the future of these technologies in the region.

Photocatalytic Reforming of Lignin for Production of H2 and Value-added Chemicals

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Abstract Ref Number from the website: ID- 5751
Session: Materials: Green Energy

ABSTRACT

Hydrogen (H2) is considered as the most efficient (Higher heating value, HHV = 141.8 MJ/kg) and clean (zero carbon emission after combustion) energy carrier which can be used in many applications such as transportation and electricity generation. Currently, H2 was mainly produced from non-renewable routes of steam reforming of hydrocarbons (e.g. methane) which are associated with significant carbon footprint (due to the high energy demand for reforming reactions and production of carbon dioxide, CO2, as the by-product). Therefore, sustainable alternatives for renewable H2 production are urgently needed to answer the ever-increasing energy demand, as well as mitigating the environmental impact. Solar-driven photocatalytic reforming of biomasses (such as cellulose and lignin) at ambient conditions presents a promising solution to produce renewable H2 due to the use of (i) biomass (which is widely abundant in nature, sustainable and, theoretically carbon neutral) and (ii) solar energy (i.e. ultimately, sun as the largest energy resource derive the catalysis).

Current photoreforming processes mainly employ cellulose and bio-derived chemicals such as bioethanol. Comparatively, although it is very challenging, the direct use of lignin for H2 production via photoreforming can be more beneficial and advantageous since it is the most abundant aromatic polymer on the earth. In addition, lignin can also be photodegraded into useful chemicals, which are conventionally obtained from fossil resources. This study aims at developing novel and efficient catalytic systems to progress catalytic photoreforming of lignin over platinised TiO2. The Pt/TiO2 photocatlysts were prepared by a wet-impregnation and photo-deposition method and characterised comprehensively by BET, XRD, UV-Vis, ICP, TPR and TEM. Lignin-derived compounds (such as phenol, vanillin, guaiacol, and vanillin methyl ether) and lignin was photoreformed at ambient conditions under UVA light in a pH-neutral aqueous solution for H2 production.

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Detection of the Scale in Oil Industry Pipelines using γ Mobile System

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Abstract Ref Number from the website: ID- 3890
Session: Materials: Green Energy

ABSTRACT

The development of the scale in the industrial oil pipeline and equipment is a common problem where the deposition of the scale will lead to reduction in the production, corrosion, and cost for repair and maintenance of the equipment and the pipelines. Different types of scale formed in the surface of the industrial oil pipelines and subsurface of equipment in the form of calcium, barium, strontium sulfate, calcium carbonate, organic and inorganic materials. Therefore, it requires a tool for early detection, to identify and quantify the thickness of the pipeline and the scales in order to protect the equipment and pipeline, minimize the cost of repair and maintenance, and prevent the shutdown of the operation. Advance measurement techniques such as gamma ray dosimetry (GRD), X-ray, computed tomography scan, and traces are widely used in different applications in laboratory. These techniques used in monitoring and diagnosis; in studying hydrodynamics of reactors, multiphase reaction, optimization of the process, scaling up the chemical processes, corrosion, agriculture, food, and water resources. The objective of this study is to develop a tool based on gamma ray mobile system for detection and quantify the thickness of the scale layer inside the service of the pipelines. The system is composed of a 137 Cs radioactive source and a NaI (Tl) scintillation detector. The source and the detector will be positioned in a geometry to make transmission measurements for efficient detection and quantification of materials inside pipelines.

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR FOURTH INDUSTRIAL REVOLUTION SESSION

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
The Gulf International Hotel, Kingdom of Bahrain
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Design, Development, and Validation of the World's First Autonomous Downhole Robot for Production Logging Operations.

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Abstract Ref Number from the website: ID-5683 Session: Fourth Industrial Revolution

ABSTRACT

A novel solution is introduced that will revolutionize intervention and production logging operations in the oil and gas industry. The design of the world's first un-Tethered Autonomous Downhole Robot (ADR) technology is discussed, starting from the early ideation phase, followed by the research and development stages, and ending with testing and validation phase.

The ADR design, consists of multiple sub-systems that will be introduced, with a special focus on the steering and navigation sub-system, the mobility sub-system, and central processing and power sub-systems.

In addition to the detailed design, the development, validation, and successful testing results of generation Zero ADR rapid-prototypes is displayed, and analyzed. The ADR managed to mobilize and maneuver through an entire test-set that included production tubing, open hole and washout environments, as well as successfully passed through restrictions.

The improvement plans to develop and demonstrate an integrated prototype robotic technology focusing on the highest risk subsystems Navigation, mobility, and Central Processing Subsystems is revealed.

The project clearly demonstrated that the ADR technology will enable overcoming the limitations associated with the current well accessibility, and reach in multi-laterals, and extended reach wells around the world. The autonomous downhole robotic platform would be able to navigate, monitor and log those wells helping eliminating the dependency on conventional intervention methods, ensuring operations safety, cost efficiency, reducing CO2 emissions, and maximizing production.

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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Arabian Gulf Seawater Profile at Qurryah Sea Water Plant

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Abstract Ref Number from the website: ID- 3857 Session:Fourth Industrial Revolution

ABSTRACT

In this paper, a study was conducted to assess the pollution level of the Arabian Gulf Sea by examining the Total Coliform bacteria populations and Petroleum Hydrocarbons contaminations in correlation with the other physicochemical properties of the Arabian Seawater at Qurryah Sea Water Plant (QSWP). Total of 15 water samples were collected, 5 samples from each zone, at an interval of one month between each batch: Zone A (Intake Channel), Zone B (Discharge), Zone D (Discharge) at QSWP, starting from June through August 2019. The following instruments have been utilized to perform the analysis required for this study: 7800 ICP-MS instrument for metals analysis, Colilert from IDEXX to quantify both the total coliform and Escherichia coli (e-Coli) bacteria, Eracheck eco (Mid-IR Laser Spectroscopy) from eralytics to measure the Oil & Grease and Total Petroleum Hydrocarbons concentrations, SPE-DEX ® 5000 Automated Extraction System from Horizon technology to extract the hydrocarbons from the seawater samples, Mettler Toledo T90 Auto-Titrator for carrying out the Chloride analysis, and ORION model 162 for measuring the conductivity of the Qurryah seawater samples. Zone D (Discharge) showed the highest Total Coliform concentration (Max.: >1600 MPN/100 mL), while Zone A (Intake Channel) was the second highest of the Total Coliform concentration (Max.: 866 MPN/100 mL). QB (discharge) exhibited the lowest contamination of the Total Coliform with (Max.: 225 MPN/100 mL). There was a clear association between the Total Coliform index and Total Phosphate & Conductivity. The relationships was established and confirmed via a powerful K-means Algorithm, a prominent tool in computer engineering, was employed to partition the dataset into distinct and non-overlapping subgroups or clusters.. The study found out that the data clustering technique can be applied to identify the sample's source. Ultimately, the study showed that the Arabian Gulf is highly vulnerable to the fecal contaminations which may be attributed to the urban sprawl and industrial revolution near the Arabian Gulf Sea.

Machine learning techniques for faster data handling in an analytical lab

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Abstract Ref Number from the website: ID- 4548 Session: Fourth Industrial Revolution

ABSTRACT

The development of innovative materials is a concerted action between several disciplines. Together with the chemical effort, physical and analytical ones are necessary to determine the characteristics and properties of the newly synthesized species.

X-ray based techniques can be ideal tools for a quick and accurate analysis of several aspects of a material. Modern X-ray diffraction techniques are able to provide quantitative information about chemical purity and atomic arrangement (structure), as well as information on the microstructure, such as shape and size distribution of the crystallites, type and quantity of lattice defects, and orientation of the crystallites. When exploited at large scale facilities (e.g., synchrotrons, neutron sources, X-ray Free Electron Lasers), diffraction can also help in fast screening (tens of thousands specimens handled and analyzed automatically), for in situ and in operando analyses (e.g., during synthesis, transformation, in operation), to obtain volumetric phase information (diffraction tomography) or provide further unexpected data (e.g., activation energies, short and long range order). The simultaneous availability of complementary techniques (e.g., Raman or FTIR spectroscopy), further widen the range of applications.

These advanced tools, with or without the support of artificial intelligence, can improve the capability of the chemist for faster development of a material possessing new or improved properties.

Some basic information and practical application cases will be illustrated and discussed.

Applying Quantitative Structure Property Relationships (QSPR) to predict Hot and Cold Properties of Middle Distillate fuels

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Abstract Ref Number from the website: ID- 6306 Session: Fourth Industrial Revolution

ABSTRACT

Nowadays many scientists came out with machine learning (ML) program to aid in prediction of new substances or molecular structures. (QSAR) Quantitative Structure Activity Relationship and (QSPR) had been developed interchangeably to handle big data in various discipline.

In line with SATORP commitment in supporting digitalization era, laboratory has taken an initiative to apply QSPR methodology to enhance efficiency and optimization. QSPR is a powerful analytical method for breaking down a thermodynamic series of numerical values describing its relevant chemical and physical properties such as Density, Boiling Point, Flash Point, Cloud Point, Pour Point and Freezing Point. Using fundamental insights about boiling range-Hot and Cold properties interactions, it can also create specialized numerical descriptors that calculate the favourable hot and cold properties and then use them as input values for a predictive model.

In order to convert these numerical descriptors for predictive model, Unscrambler program has been used that first select relevant variables from the pool of descriptors and then used either linear or non-linear operations to combine selected descriptors into a predictive model. With a proper correlation and validation program, precise data for hot and cold properties of middle distillate fuels can be achieved. This approach could be a backup to on-stream analysers, advance process control as well as laboratory efficiency and optimization.

Case study for new quick measurements of oil in waterf from GOSP usinglaser induced floresene based technology

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Abstract Ref Number from the website: ID- 6404 Session: Fourth Industrial Revolution

ABSTRACT

Oil and gas industry generate certain amount of water from different processes such as GOSPs. Gas, oil and water separate into three different streams for further processing. Water is re-injected into reservoir to maintain the pressure and drive oil out. In some cases, some oil carry with Water stream to reinjection but there are limitations on the quantity of oil due to environment regulations and reservoir specification. The oil in water should not exceed more than 100 ppm in reinjection process.

A new technique that will give results in a shorter time with lower cost and easier to use was utilize to measure oil in water in multiple GOSP in SA. The portable analyzer gives higher accuracy in lower range, requires no solvents and consumable. In addition, the analyzer utilizes the Laser Induced Fluorescence Spectroscopy technology and was validated using UV-visible Spectroscopy in R&DC. The results comparing the application of this analyzer with UV-visible Spectroscopy.

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Artificial Intelligence for Predicting Multiphase Flow

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Abstract Ref Number from the website: ID- 5682 Session: Fourth Industrial Revolution

ABSTRACT

Multiphase flow metering is an important tool for production monitoring and optimization. Although there are many technologies available on the market, the existing multiphase meters are only accurate to a certain extend and generally are expensive to purchase and maintain.

Virtual flow metering (VFM) is a low-cost alternative to conventional production monitoring tools, which relies on mathematical modelling rather than the use of hardware instrumentation. Supported by the availability of the data from different sensors and production history, the development of different virtual flow metering systems has become a focal point for many companies.

This paper discusses the importance of flow modelling for virtual flow metering. In addition, main data-driven algorithms are introduced for the analysis of several dynamic production data sets. Artificial Neural Networks (ANN) together with advanced machine learning methods such as GRU and XGBoost have been considered as possible candidates for virtual flow metering. The obtained results indicate that the machine learning algorithms estimate oil, gas and water rates with acceptable accuracy. The feasibility of the data-driven virtual metering approach for continuous production monitoring purposes has been demonstrated via a series of simulation-based cases. Amongst the used algorithms the deep learning methods provided the most accurate results combined with reasonable time for model training.

Development of Materials for additive manufacturing

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Abstract Ref Number from the website: ID- 5400 Session: Fourth Industrial Revolution

ABSTRACT

Additive manufacturing (AM) is gaining increasing importance in industry not just as a technology for prototyping but also, and in most cases, for the production of functional parts in different fields.

Successful additive manufacturing with plastic resins and compounds depends on selecting the right material for the process, design, and end-use application. Although additive manufacturing is advancing rapidly on multiple fronts with the goal of expanding from a prototyping/limited production method to a robust, reproducible manufacturing process, optimized materials have been limited to date. The primary reason is that additive manufacturing differs significantly from classic processes such as injection molding, and therefore requires specialized resins and compounds tailored to provide the desired properties.

In this study, main characteristic of resin/compound for AM processes that can meet the higher performance demands of production parts in the end-use environment will be explored.

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Machine Learning to Predict Boiler blow Down pH

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Abstract Ref Number from the website: ID-4482 Session: Fourth Industrial Revolution (IR 4.0) -- Artificial Intelligence

ABSTRACT

Alkalinity is a measurement of dissolved alkaline substances in water. It quantifies the water's ability to neutralize acid. To control alkalinity levels in boiler water, hydroxide level is raised to increase pH and therefore maintain anti-corrosion layer (magnetite) at the equipment metallic walls.

In this paper, we are going to explore and use different sized boiler historical data and try to utilize machine learning models to predict the pH of boiler blow and possibly feed water as well as return condensate. using large-scale unstructured multi-source data, machine learning can accurately predict leaching behavior, predict missing data, and time forecast. The accuracies of the four machine learning models used in this paper were higher than 80.0% for predicting the pH of boiler blow down water samples

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR GREEN ENERGY SESSION

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PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR WATER PURIFICATION AND WASTE MANAGEMENT SESSION

Synthesis of Flash Graphene from Plastic Waste

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Abstract Ref Number from the website: ID- 6185
Session: Materials: Materials for Environment and Wastewater Purification

ABSTRACT

Plastic waste pollution is one of the challenging environmental concerns we are facing today. In this presentation, I will show how the flash Joule heating (FJH) method enables the transformation any carbon source, including plastic waste, to high-value flash graphene (FG). Other carbon sources that can transformed into graphene are petroleum coke and carbon black. Based on the nature of the carbon source, the electricity mode is adjusted interchanging between alternating current (AC) to direct current (DC) to have a successful flash. The FJH technology is highly economical, costing as low as $30 ton-1 of waste to process. The graphene produced by the flashing method is turbostratic and can be easily processed into composites. In addition, I will discuss some of the large-scale potential applications of flash graphene in building materials and plastics composite industries.

Utilization of both Agricultural and Plastic Wastes for Packaging Applications

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Abstract Ref Number from the website: **ID- 6188**
Session: Materials: **Materials for Environment and Wastewater Purification**

ABSTRACT

The exploitation of recyclable, natural and environment friendly materials is rapidly increasing for various industrial applications. These materials include both agricultural and plastic wastes. This is due to certain characteristics such as abundance, ease of processing, low density and cost as well as environmental conservation. In this project, efforts have been made to take advantage of such wastes. Palm residues (trunk) were cleaned, grinded to micro/nano-scale sizes using a mechanical treatment. This reduction into these very small sizes without any chemical treatment is feasible choice from both commercial and environmental point of view. On the other hand, plastic water bottle caps cleaned and then recycled mechanically to be mixed with treated trunk. The waste materials compounded together using an extrusion process followed by hot press technique at optimized processing conditions. Thermal and mechanical properties of obtained composite materials characterized by a wide range of analytical and testing techniques. The results showed that the initial thermal decomposition of composite materials > 180 oC, tensile strength ~ 30 MPa and the tested films showed no liquid permeability during 60 days. These results indicate that the investigated composite materials could be utilized as general packaging materials.

Efficient Nanomaterials for Oil Removal: Toward Produced Water and Wastewater Purification

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ABSTRACT

The objective of this work was to prepare and test new nanomaterials based on modified carbon nanostructures including carbon nanofiber grafted with polystyrene foam for efficient oil and water separation. The nanomaterials were prepared via the method of in-situ polymerization. The polystyrene foam was chemically treated with acetone to accomplish a temporary soft structure, which allows for good interaction and incorporation with carbon nanofibers. Introducing the carbon nanofibers provided micro- and macro-porous cavities, which enhance the oil removal efficiency. The prepared nanomaterials were characterized by using different techniques such as scanning electron microscopy (SEM), contact angle analyzer, and BET. Various composites were synthesized by changing the ratio of carbon nanofibers to polystyrene. The material revealed superhydrophobic and oleophilic characteristics for the adsorption of several oil compounds. This could have been due to the growth of the polystyrene chains on carbon nanofiber as indicated by the SEM images. The ratio of carbon nanofiber to polystyrene was changed to get the optimum ratio with the highest removal of oil from water. The optimum combination of carbon nanofiber with polystyrene was a 1:5 ratio. The carbon nanofiber interaction with styrene significantly improved the contact angle from around 74˚ to more than 150˚ and the surface area from 14 to 139 m2/g for the prepared optimum ratio. The nanomaterials were evaluated for the separation of the heptane and n-decane from the water. It showed a complete separation of organic compounds from water. The material displayed an increase in adsorption capacity with increasing hydrocarbon molecular size. The adsorption rate of n-decane was relatively slow compared to heptane due to the larger molecular size filling more porous cavities in the material structure. The nanomaterials demonstrated a satisfactory recyclable capability after multiple uses. The incorporation of polystyrene into carbon nanofiber displays potential for reducing oil contamination, and it is an effective way to cope with environmental pollution. It is efficient and cost-effective, and can be produced easily on a large scale. This makes it a promising material for both produced water treatment and offshore oil spillage cleaning.

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Advanced Laboratory Methodology to Evaluate Friction Reducer for Slickwater Unconventional Fracturing

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Abstract Ref Number from the website: ID- 4112
Session: Materials: Materials for Environment and Wastewater Purification

ABSTRACT

Slickwater fracturing has increased over the past couple of decades in the development of shale and tight formations. Friction reducer is the main component of slickwater, which reduces drag in the tubular. For successful and economical slickwater hybrid fracturing treatment, selection and optimization of friction reducers, plays a key role. This paper presents a new insight into optimizing friction reducer using helical coiled flow loop at high-pressure, high-temperature (HPHT) conditions.

Usually, friction pressure is estimated by pumping slickwater fracturing fluid through a straight tube and measuring differential pressure across the tube. This requires pilot-scale laboratory setup and testing at HPHT, which can be challenging. In this paper, a smaller size equipment, helical coiled flow loop was utilized to estimate friction pressure of slickwater fracturing fluid. Friction reducers can be rigorously tested for degradation because secondary flow resulting from centrifugal forces can be caused by the coil curvature. Correlations for the Darcy friction factor as a function of Reynolds number has been developed for helical coiled fluid loop in both laminar and turbulent flow regimes. The present study evaluates different friction reducers in a ¼ in. ID smooth helical coiled flow loop. The correlation developed for Darcy friction factor was well validated for water with data available from literature. Polyacrylamide based friction reducers with different concentrations were used in this study. The friction pressure, with and without friction reducers, was compared at different flow rates. Percent drag reduction at different polymer concentration was also evaluated using helical coiled flow loop. Thermal degradation of friction reducers was evaluated by varying temperature up to 300°F. Dropped drag reduction due to secondary flow resulting from centrifugal forces in helical coil can judge friction reducer more thoroughly than with a conventionally used straight tube flow loop.

Evaluation of Foam-Gels for Conformance Control in High Temperature High Salinity Carbonates

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Session: Materials: Materials for Environment and Wastewater Purification

In naturally fractured reservoirs, conformance control prior to EOR application might be essential to ensure optimal contact and sufficient sweep.Recently, few studies investigated combining foams and gels into foamed gels. Foamed gels have been tested and proven in some fields. However, very limited studies were performed at high temperature and high salinity, and none in carbonates. In this work, we study the potential of foamed gels for high temperature and high salinity carbonates.
In this work, we rely on bulk, micromodel, and core-scale tests. Bulk tests were used for initial screenings. Five solutions were prepared with different concentration ratios of foamer to gelant. A shaker was used to generate foam inside the test-tubes. Image analysis was used to record foam heights. Height were used to screen foaming agents and to study gelant effects on foamers in terms of foam strength (heights) and stability (decay). Moreover, the effect of foamers on gelation time and gel strength was evaluated through bottle tests, and rheological measurements, respectively. To further evaluate foam/gel synergestic effects, micromodel tests were performed. Based on the results, an optimal concentration ratio was determined and used in core-scale displacements, to further evaluate the hybrid process EOR potential.

Bulk results suggested that addition of the gelant up to a 2:1 foam to gel concentration ratio has minimal effect on the foam. However, gelation time was slightly delayed after the addition of the foaming agent and the gel was stronger. In micromodels, waterflooding recovered about 40% OOIM (original oil in micromodel). A foamed/gel process followed by chase waterflooding recovered an additional 15% OOIM. In this foamed/gel process and for the micromodel experiments, the foamed gel was firstly injected. The foam lamellas started to collapse after about two minutes. About two hours later, the foamed/gel started to crosslink and a gel started to form. Consistent results were observed in coreflooding. The initial waterflood yielded a recovery of 48% OOIC (original oil in core). After foamed/gel injection, the chase waterflood resulted in an additional recovery of about 17% OOIC.

Effective conformance control is critical to the success of EOR applications in mature and naturally fractured reservoirs. Combining two of the most widely used conformance control methods (foams and gels) can yield enhanced and sustainable conformance control. Our laboratory results demonstrate that such synergetic conformance control can be achieved in high salinity and high temperature carbonates with pronounced impact.

Synthesis and Modification of Mesoporous Carbon Surface for the Quick Removal of Metal Ions

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Session: Materials: Materials for Environment and Wastewater Purification

ABSTRACT

Inexpensive functionalized porous carbon (PC-KF) as a sorbent was prepared from less useful petroleum matrix leftover and characterized by several analytical and spectroscopic methods. The sorbent used for the removal of several heavy metal ions from the aqueous solution. The optimized conditions were applied: concentration 0.5 mg/L, contact duration 6 minutes, dose of adsorbent 0.3 g/L, pH 8.0, and ambient temperature 25 ºC. The removal was very fast, with a maximum amount of 95.5% (1.59 mg/g). The sorption followed Freundlich, Temkin, and Dubinin-Radushkevich isotherm models, indicating multilayers sorption on the heterogeneous surface. The free energy (ΔG°) values have good range at 20ºC, 25ºC, and 30 ºC. The enthalpy (ΔH°) and entropy (ΔS°) values represented adsorption process is spontaneous as well as exothermic due to both negative values. In most of the metals, the kinetics of the adsorption process was concluded to be pseudo-second-order. The sorption process worked at optimized time and pH and, therefore, this method can be considered a fast removal of heavy metals ions with the economy. Henceforth, the present method, based on the functionalized porous carbon, could be a good candidate for efficiently removal of heavy metal ions from polluted water.

The authors would like to acknowledge the support provided by the Deanship of Scientific Research (DSR) at King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, Saudi Arabia.

Enhance the Rolling Resistance of Natural Rubber via Silicone Chemistry Reagent and Study its Rheological Properties

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ABSTRACT

Natural rubber (NR) has been preferable to its counterpart synthetic due to the remarkable mechanical properties and as a greener alternative material to the synthetic rubber. Rolling Resistance (RR) enhancement is desired to minimize carbon dioxide ($CO2$) emissions produced via vehicle footprint. A reinforcing silica filler without any incompatibility among silica molecules and NR particles has shown to enhance the silica/polymer interactions within NR, leading to lower the rolling resistance. Silica has proved to improve the mechanical properties such as tensile strengths and toughness, resulting in green NR tires, that has potential to replace synthetic rubber.

In this work, the impacts of silica to the micro-structure of NR, the crosslinking process, and the rheological properties of NR are investigated through numerous approaches. Characterization of the network structure and aggregates formed in NR micro-structure due to silica addition are determined via optical microscope and scanning electron microscope (SEM). The fractal dimension of different aggregates size formed via addition of silica is calculated using MATLAB image processing. Various types of surfactants are examined to stabilize the NR with silica and observe the rubber particles response. Rheological properties of concentrated NR and viscoelastic properties of NR with silica addition are carried out through ARES-G2 rheometer. Results displayed in this work are manifested that silica reinforced NR can form a robust network. Sodium Dodecyl Sulfate (SDS) surfactant is tested effectively to provide a stability in NR structure without forming

aggregations. The rheological results are demonstrated the various viscoelastic behavior of NR with manipulating silica amount addition.

Acknowledgments. This work was a result of various research groups collaboration headed by Tom Rosenmayer, founder of Silpara Technologies LLC. Silparatech.com. Thanks & appreciation are extended to National Science Foundation (NSF) for the financial support. Moreover, gratitude is given to Kuwait Institute for Scientific research, KISR on the encouragement and support.

Degradation of Ammonia in Aqueous Solution Using a Pilot-Scale Advanced Fenton-Based Electrochemical Oxidation Unit

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High levels of ammonia in aqueous solution is considered serious environmental and health problems if not adequately treated before disposal because it leads to the formation of harmful nitrite and nitrate ions. Current treatment methods usually suffer from several shortcomings including sludge formation and high cost and the search for advanced treatment technologies are still going on. The study aimed to remove ammonia and its associated degradation by-products using a pilot scale unit with an undivided plate and frame cell, provided with a Boron-doped Diamond (BDD) anode and a carbon-Polytetrafluoroethylene (PTFE) gas diffusion electrode (GDE) as cathode, in a batch recirculation mode. The effects of various treatment conditions on ammonia degradation, including pH, E-conductivity, current density, feed flow rate, and iron (Fe2+) dosage. Results showed that increasing the chloride content of water via increasing the conductivity and the current dosages had the greatest effect on ammonia degradation, while Fe2+ did not have any effect. Results also showed that the optimum operating conditions favorable to complete ammonia degradation were- 60 mA/cm2, pH 7.5, 0.4 m3/h water circulation rate and water electrical conductivity of 43,300 µS/cm- within 2 hours for BDD anode. Ammonia degradation by-products (nitrate, NO3- and nitrite, NO2) were identified and measured during the treatment with NO2- ions being totally eliminated after 15 min of treatment while NO3- ions were formed after one hour of treatment, reaching at optimum operating conditions a concentration of 50 mg/L.

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PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR ADVANCED LABORATORY METHODOLOGIES SESSION

Advanced molecular characterization of vacuum gas oil (VGO) using comprehensive two-dimensional gas chromatography

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Session: Advanced Laboratory Methodologies

ABSTRACT

Clean fuel legislation in Europe, America, Asia and Middle East is driving the demand for low sulfur diesel (LSD) fuel. The concurrent increasing demand of transportation fuels leads refiners to produce ever cleaner transportation fuels. In this tense energetic context, the improvement of existing refining tools and the development of new processes has become a key issue. In parallel, the absence of analytical tools able to comprehensively characterize feedstocks and corresponding products at the molecular scale has become an obstacle to the development of efficient catalysts and accurate kinetic models.

Owing to a higher resolution power and an enhanced sensitivity, comprehensive two-dimensional gas chromatography (GC×GC) has been implemented to improve the characterization and identification of both hydrocarbons and sulfur species occurring in vacuum gas oil sulfur compounds. Key GCxGC parameters include injection and separation. Combining GCxGC with various detectors (FID, SCD and qMS), the comprehensive characterization (identification and quantification) of hydrocarbons and sulfur species by class could be achieved. To that end, GCxGC was applied to investigate VGO samples resulting from different processes. The individual simulated distillation curves have also been established for all studied samples without limitation in terms of matrix. Comparison of results with existing normalized methods demonstrated the power of GCxGC over conventional molecular characterization techniques, showing that GC×GC should become an essential tool for advanced sulfur speciation analysis of VGOs.

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Data Stitching for Micro Crude Assays. Part III: Heavy Ends

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Abstract Ref Number from the website: 4494

Session: Advanced Laboratory Methodologies

ABSTRACT

The development of hydrocarbon conversion technologies benefits immensely from comprehensive compositional knowledge of feedstock, intermediate, and product streams. For industrial scale processes, such information can be obtained using crude assay, including fractionation by distillation and routine tests, in addition to advanced analytical speciation of the fractions. Data can then be recombined based on the distillation yields. In early technology development stages, the low sample volume (too little for distillation) has been a limiting factor for achieving a comprehensive, detailed quantitative analytical characterization. In this work, consisting of three parts, we show the use of simulated distillation to quantitatively "stitch" together different data sets, obtained using speciation techniques, with minimal sample volume requirements.

In particular, heavy ends characterization for wide boiling range samples (such as crude oils, or heavy fuel oils) is available for small sample volumes, but an unknown portion of the lighter components is omitted in the analysis. Additional information, specifically the physical distillation yield of the heavy ends fraction in question, is required for merging such data with light ends characterization into a complete sample description. In this 3rd installment of the work, we overcome this issue through the development of a model to determine the boiling curve solely on FT-ICR MS information on heavy ends components. The new boiling curve description, together with simulated distillation (SIMDIS), allows to quantitatively "stitch" together the different data sets into a continuous model of composition.

The new model predicts the boiling properties for heavy petroleum components, from data produced using atmospheric pressure photo ionization (APPI) Fourier transform-ion cyclotron resonance mass spectrometry (FT-ICR MS). Experimental validation was achieved through state-of-the-art FT-ICR MS analyses of narrow boiling range fractions, and was corroborated through thermodynamic calculations to outline the impact of molecular structure on component boiling points. The combination of the quantitative dimension of simulated distillation with the unmatched resolution of FT-ICR MS opens a new pathway towards detailed compositional knowledge on wide boiling hydrocarbon samples, while minimizing sample volume requirements

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CHARACTERIZATION OF SLUDGE DEPOSITS IN SOUR GAS PIPELINES AND MITIGATION PLAN TO MINIMIZE BLACK POWDER FORMATION AND PIPELINE BLOCKAGE.

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Session: Advanced Laboratory Methodologies

ABSTRACT

This technical paper describes characterization of sludge deposits — from a Saudi Aramco sour gas pipeline — using advanced analytical techniques. The accumulated black powders affect the integrity of the pipeline and choke the filters at the receiving end. The findings will help the investigation team to identify the nature of the deposits, and establish a mitigation plan to minimize black powder formation and pipeline blockage. The thermogravimetric analysis results of the as-received sludge deposits, revealed that the organic contents are 98.32 wt% and 95.59 wt% for sludge deposit samples from the pipeline and trap. The corresponding inorganic crystalline material concentrations are 1.68 wt% and 4.41 wt% for these two samples. The challenge of the X-ray powder diffraction (XRD) study is to get the accurate phase identification and quantification of the very small quantities of the inorganic crystalline part of these complex sludge samples. The XRD results revealed that these tiny inorganic crystalline samples mainly consist of sulfur [S], which are supported by the X-ray fluorescence results. The findings will help the investigation team to determine the root cause of the deposits, and establish a mitigation plan to minimize black powder formation and pipeline blockage.

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Root Causes Analysis for Preliminary Failure and Deposit Material

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Session: Advanced Laboratory Methodologies

ABSTRACT

The sludge and solid deposits that frequently accumulate inside the equipment used in the oil industry can cause failures and temporarily shut down refinery and gas plants. Selecting unsuitable materials, conditions, and chemicals can also cause preliminary failures and shut down plants. In this paper, advanced instruments (FTIR, TGA, DSC, GCs, NMR, ESEM, and XRD) were used to characterize deposit samples to identify the root causes of failures, and the composition of the deposit samples. The goal is to use this information to develop corrective action that can prevent failure reoccurrence. FTIR, NMR and GCs have been used to study the organic parts, and XRD, TGA, ESEM and DSC have been used to study the inorganic parts. The results showed that main reason for the preliminary failure was improper material selections and treatment conditions. Also, the results indicated that the main source of the deposits was carry-over of heavy hydrocarbons, due to the upset in the plant process or corrosion products.

The paper will present the applications of these advanced instruments for performing failure analysis to identify the sources of the failure, deposit materials, and composition of the deposits. The paper will also elaborate on the importance of obtained data for selecting the desirable materials and optimum plant conditions, as well as understanding the reaction mechanisms. Additionally, the in-house advanced materials characterization obtained from XRD, TGA, ESEM, and DSC techniques will be described in this paper.

GCMS-SIM a powerful tool for low level quantification in complex hydrocarbon mixture

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Session: Advanced Laboratory Methodologies

Abstract

GC and GCMS are one of the core pillars for the analysis of hydrocarbons. In fact, it is one of the most used techniques for the analysis of hydrocarbons. The advantage of GC-FID (Flame ionization detector) to ionize the hydrocarbon and its huge linear range has helped GC to become one of the most preferred techniques in hydrocarbon analysis. However in the presence of unknown samples GC-FID faces challenges of identification of unknown compounds or compounds eluting at the same retention time. This is where GCMS plays the upper hand as it can be used for identification of unknown. The mass spectrometer, which is used as the detector in the GCMS, can be used in two ways. One is for Scan or total ion chromatogram (TIC) mode in which it monitors all the ions in the mentioned range. For example if the mass spectrum is set to monitor m/z of 20 to 400, it will monitor everything within the range. The other mode of operation the mass spectrum is single ion monitoring (SIM) or single ion mode. This unlike the TIC is used to monitor a single or few specific ions. The advantages of GCMS, SIM over TIC is it can be used to search for specific compounds in a cluster of several compounds. As SIM uses only one or few ions, it has enhanced sensitivity. SIM can also be used in cases where peaks are overlapping.

The current paper describes on how GCMS-SIM mode has advantages in analysis for direct injection as well as using headspace with specific examples. In one such examples, the authors discuss on how an alcohol can be quantified in a mixture containing large number of hydrocarbons, especially when it is co-eluting with some of the peaks of the hydrocarbons. One of the critical things in the SIM mode is to use an ion, which has strong signal, quiet often the base peak until other compounds also have similar ions. The second example discussed here is on quantification of oxygenates in the hydrocarbons using a single column. The other examples discussed by the authors are based on using headspace GCMS in SIM mode. In one of the two examples, the authors discuss on the challenges of quantifying BTX (Benzene, toluene and Xylene) in polyethylene and how GCMS in sim mode can be used to do so in a much simpler way.

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GAS OIL CHARACTERIZATION USING MULTI-DIMENSIONAL GAS CHROMATOGRAPHY, A TOOL TO IMPROVE THE REFINING PROCESSES.

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Session: Advanced Laboratory Methodologies

Abstract

Crude oils are playing a critical role in securing the world's ever-growing need for fuel and petroleum products. Heavy crude oils are likely to play an essential role in securing the world's growing demand for energy in the near future.

The refiners are not able to determine the processability of the crude depending on crude oils' basic properties such as API gravity and sulfur contents. On the other hand, heavy crude oils processability assessment requires in-depth compositional information to understand the chemistry of refining processes. This paper presents the results of a comparative study of two straight run gas oil fractions of Kuwaiti heavy crude oils from different reservoirs but with similar basic properties. The emphasis of this study is on the molecular composition of these gas oils to determine the molecular differences between them, with a detailed discussion of the experimental procedures used in this study. The composition of the gas oil fractions was analyzed with a two-dimensional gas chromatograph system utilizing a thermal modulator and equipped with a flame ionization detector (FID) and sulfur chemiluminescence detector (SCD). Due to the importance of the sulfur compounds on the gas oil processability, this study focuses on identifying the sulfur compounds, which are typically part of large molecules that vary between different crude oils. These larger molecules can be chemically different, as some can be very reactive while others are stable or even inert towards catalytic reactions. Thus, it was essential, from the processor point of view, to identify and quantify the different chemical species of sulfur present in petroleum products. Such information is essential for downstream processes and should help in the development of improved catalyst systems for the heavy crude oils.

Combining Gel Permeation Chromatography and FT-ICR MS for Crude Oil In-depth Characterization.

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Abstract

To enhance oil production and optimize refining operations, a clear understanding of the complex structural composition of crude oil is needed. Combining two or more analytical techniques amplifies the strength of each technique, and avails new information about the composition of the studied crude oil. In many cases, chromatography techniques are coupled with high-resolution mass spectrometry for a comprehensive characterization of hydrocarbon and heterocyclic components. Chromatography plays a vital role in decreasing the complexity of crude oil samples, while mass spectrometry reveals structural information of thousands of different species present therein. One of the chromatography techniques that has been successfully applied to petroleum samples for determining boiling point distributions of heavy fractions, and for reducing the sample complexity before characterization by mass spectrometry, is gel permeation chromatography (GPC). Therefore, we have employed GPC for the fractionation of crude oils, to separate the components based on the average number of alkyl carbon atoms, followed by ultrahigh resolution mass spectrometry for subsequent characterization.

Here, we demonstrate the universality of the method for separating aromatic compounds based strictly on the number of alkyl carbon atoms for five different crude oils with different properties. The presentation will cover the parameters of the GPC fractionation and characterization by Fourier transform-ion cyclotron resonance mass spectrometry (FT-ICR MS), calculation of alkyl carbon atom number for the separated GPC fractions, and a detailed discussion of the results for a variety of compound classes, as well as data for crude oil of different geographic origin. As a result we can show new insights into the molecular composition of Arabian and other crude oils.

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Application of Gas Chromatography-VUV for the composition analysis of complex sample matrices in Refinery & Petrochemical Industries

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Abstract

Gas chromatography with vacuum ultra violet spectrometer is a recently developed state of art powerful analytical tool that could considered as a laboratory workhorse for the compositional analysis of light and middle distillate hydrocarbons. The unique and novel capabilities of VUV spectroscopy overcome the issues associated with the conventions GC techniques with FID detection. The resolution issues of closely and co-eluting compounds were resolved by VUV spectral deconvolution techniques. A detailed correlative study been carried out and ensured its efficiency, versatility, suitability for unknown sample matrices with less run time, opex and capex expenditures. Furthermore, the versatile technique has a potential to replace most of the conventional GCs and the respective test methods for petroleum product certification.

Novel In-Situ Characterization of Rock-Fluid Interfaces using Transmission Electron Microscopy

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Session: Advanced Laboratory Methodologies

ABSTRACT

SmartWater flooding, through tailoring of injection water salinity and ionic compositions, has been demonstrated as a promising technology to increase oil recovery in carbonate reservoirs. The favorable change in wettability from oil-wet to more water-wet is identified as one main consequential effect responsible for enhanced microscopic scale displacement efficiency observed in SmartWater flooding. However the causative interaction mechanisms occurring at rock-fluid interfaces leading to this wettability change are not yet fully understood. To address this gap, several conventional macroscopic scale methods such as coreflooding, contact angle, surface charge and interfacial tension (IFT) were widely used in the existing knowledge. Since such interaction at rock-fluid interface occurs at molecular scale, the conventional methods fail to provide sufficient information due to limited resolution and visualization capabilities. Therefore, it becomes challenging to understand the behavior of fluid interactions with carbonate minerals at molecular scales.

To overcome the aforementioned challenge, Transmission Electron Microscope (TEM) has been identified as a novel approach because it can provide both atomic resolution and chemical distribution details at rock-fluid interfaces. Cryogenic TEM is mainly used as the liquid sample cannot be observed and characterized in ultra-high vacuum conditions. Nevertheless, cryo TEM still has an issue that the cryogenic environment is different from real reservoir conditions and the obtained results could not be representative. In this study, liquid cell TEM holder with encapsulation function features has been applied so that liquid sample can be observed and analyzed close to its native condition. Energy dispersive spectroscopy (EDS) analyses have been also utilized to provide the chemical mapping of rock-fluid interfaces. The results provide, for the first time, nano-scale images of oil droplets, calcite nanoparticles and dissolved salt ions at their native environment. Furthermore, the compositional distribution of multiple elements and elemental mapping of the structures in solution are discussed.

This novel nanoscale characterization brings a new insight about the chemical distribution of elements and characteristics of interfacial layer at rock-fluid interfaces. Such understanding becomes important to optimize the salinity and injection water compositions used for improving oil recovery in carbonate reservoirs.

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Ethylene Furnace Antifoulant Chemistry Helps Extend Two Separate Furnace Runs in the Middle East

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Abstract Ref Number from the website: ID-6295
Session: Laboratory Operational Excellence: Advanced analytical and laboratory methodologies

ABSTRACT

A Middle East ethylene cracking plant with several furnaces asked Halliburton for a chemical treatment program to increase the time between decoking operations.

Halliburton recommended their Ethylene Coke Control (ECC) product line based on a successful program operating in the Western Hemisphere.

The proper application of this design-specific chemical treatment resulted in a significant average time increase between decoke cycles. At one furnace, it increased to 58 days from 24 and to 50 days from 20 at the second.

The more than 50 percent increase in time between decoke operations allowed the operator to gain more from their ethylene furnaces by reducing downtime and increasing throughput. The life of the furnace tubes also extended beyond the period a complete retube was expected/required.

In this paper, the authors presents performance results and the design criteria of the chemistry driving the outcomes. Lessons learned during R&D are also presented as they relate to factors causing furnace fouling and how it can be remediated.

Characterization and Root-Cause Determination of Inorganic Deposits

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Abstract Ref Number from the website: ID-4099
Session: Laboratory Operational Excellence: Advanced analytical and laboratory methodologies

ABSTRACT

Determination of scale type with confidence is the first and the most important step for the development of an effective scale management program. In this work, we present a case study on root-cause determination of inorganic deposits in an electric submersible pump (ESP) system, based on the advanced instrumental analyses of scale samples. Inorganic scale deposition was determined — by a Dismantle Inspection & Failure Analysis (DIFA) study — as the main cause for the premature failure of an ESP system. Collected scale samples were characterized for chemical composition and microstructures by using the state-of-the-art X-ray powder diffraction (XRD), X-ray energy dispersive microanalysis (EDS), and environmental scanning electron microscopy (ESEM) techniques. Then the water compatibility simulation model was used to predict the scaling formation tendencies of the binary and ternary among formation water, injection water, and completion fluid. Laboratory tests were also conducted to confirm the model prediction results, and assess the effectiveness of potential chemical treatment. Study results revealed that the inorganic deposits were based on calcium sulfate, mainly in the form of gypsum. The scale precipitation was caused by the mixing of formation water or injected seawater with calcium chloride completion brine, lost into the reservoir during well workover. The efficacy of scale inhibitors was limited by incompatibility with the high calcium produced waters.

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A Novel Approach to Monitor Proppant Consolation during Hydraulic Fracturing with Dynamic Measurement: Experimental Study

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Abstract Ref Number from the website: **ID-4261**
Session: Laboratory Operational Excellence: **Advanced analytical and laboratory methodologies**

ABSTRACT

Proppants and proppant combined additive are increasingly used in screenless completions. In these applications, no screen or annular gravel pack supports the external or perforation pack. The role of the proppant pack changes from providing stimulation and reduced drawdown of the well to actually supporting the perforations. Resin coated proppant is used in hydraulic fracturing applications to stimulate oil/gas wells for production enhancement. This technology is applied in sandstone reservoirs to mitigate sand due to the reduced drawdown pressure. The objective of this study is to assess the effectiveness of the newly developed method to monitor the proppant consolidation and to provide the operator with an optimum shut-in time before putting the well back in production. A new experimental method was developed to monitor the curing process of resin-coated proppant as temperature increases. The velocity of both shear and compressional waves were being monitored as a function of temperature. The tested resin of coated proppant sample has been housed in pressurized vessel. The pressurized vessel was subjected to varying temperature profile to mimic the recovery of the reservoir temperature following propped hydraulic fracturing treatment. The role of closure stress, temperature, curing time and carrier fluids in attaining a maximum strength of RCP following a propped hydraulic fracturing treatment has been investigated. Also, the unconfined compressive strength (UCS) of various types of RCP has been measured. The testing methods currently practiced in the industry to qualify proppant for field applications are based on physical characterization of several parameters such as specific gravity of proppant, absolute volume, solubility, roundness, sphericity and bulk density. The sieve analysis, compressive strength, and API crush testing are also conducted. The API Recommended Practices; API RP 56, 58, and 60, are the main

procedures used to test proppants for hydraulic fracturing treatments. There is no API testing method for RCP; therefore, this study introduces a new testing procedure using acoustic velocity as a function of temperature, and compressive strength as a function of time to qualify a given RCP for a particular reservoir of known stress and temperature. The final outcome of this study is to come up with an established procedure to maximize the success of propped hydraulic fracturing treatment and minimize the occurrence of follow back incidents.

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR LABORATORY OPERATION EXCELLENCE SESSION

No Proceedings of abstracts received from Session Chair by 12:20 on 14 NOV 2022

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR INDUSTRIAL CHEMISTRY UPSTRAEM APPLICATION SESSION

THE *FIRST* GULF CHEMISTRY ASSOCIATION
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Rheology, Stability, and Adsorption of Two Amphoteric Foaming Agents for CO_2 Mobility Control Applications Under Reservoir Conditions

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Abstract Ref Number from the website: ID- 4323

Session: Industrial Chemistry-Upstream Applications

Foam injection is one of the most promising techniques to overcome gas mobility challenges during enhanced oil recovery processes. Foam reduces gas mobility by increasing the gas apparent viscosity and reducing its relative permeability and, consequently, improving the sweep efficiency. The stabilization of foam at reservoir conditions, together with reducing surfactant adsorption on the rock minerals are the major challenges facing this technique.

Bulk and dynamic foam tests were conducted to evaluate the effectiveness of two amphoteric surfactants, Amphosol LB and Ampholsol CG, on stabilizing foams at harsh reservoir conditions (100 oC and 57,000 ppm of brine salinity). The stability of surfactant solutions using bottle test, as well as the foam rheological properties using foam rheometer apparatus were quantified. Also, the CO2 mobility reduction as a result of foam generation was measured using two different systems: microfluidic device and coreflooding apparatus. Also, the adsorption of both surfactants on carbonate rock minerals was quantified using the coreflooding apparatus.

The experimental results demonstrate that both surfactant solutions are able to generate foams at reservoir conditions. The Amphosol LB surfactant produces foam with relatively higher apparent viscosity when compared to Amphosol CG surfactant. The results also show that Amphosol LB surfactant retains less to the carbonate rock minerals when compared to Amphosol CG surfactant. The amount of surfactant adsorbed by the rock minerals is about 0.257 and 0.315 mg/g of rock for Amphosol LB and Amphshol CG solutions, respectively. In the microfluidic chip and actual rock sample, the results also demonstrate that Amphosol LB surfactant shows higher resistance to gas flow and, accordingly, higher mobility reduction factor of CO2 when compared to Amphosol CG surfactant. Higher apparent viscosity, smaller adsorption to the rock, and greater CO2 mobility reduction are indicative of lower cost, more efficient, stronger, and more stable foam for reservoir applications.

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Fracture Cleanup Determination by Guar Measurement of Flowback Fluid Samples

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Session: Industrial Chemistry-Upstream Applications

Hydraulic fracturing is a well stimulation process used to maximize production of oil and natural gas used to both create a new fracture and to enhance insitu subsurface fracture systems to allow oil or natural gas to move more freely from the rock pores to the production wellbore. Post fracturing flowback procedure is known to be very critical in the production performance of a fractured well. An improper flowback procedure often leads to lower retained conductivity near the wellbore resulting in reduced production. Controlled flowback is beneficial for properly removing polymer gel residue from the proppant pack. The degree of propped fracture cleanup is related to a number of factors that relate to the measurement of Guar polymer contained in the fluid flowback samples.

Measurement of Guar carbohydrate from fluid flowback samples is used to estimate the amount of guar recovered after fracturing treatment. In this paper we show, in a field study and laboratory analysis, that the measurement of the Guar polymer in the fluid flowback can be used as an indication of the fracture cleanup. The Anthrone method, a technique of measuring the total guar carbohydrate in the fluid flowback samples, is used. Anthrone dissolved in sulfuric acid forms a yellow solution. In presence of guar or its derivations, the solution will turn to green/blue. Using Ultra violet (UV) spectrometry technique, guar concentration in the fluid flowback samples can be determined from the intensity of measured color. Many fluid samples collected from various fields were analyzed and results will be shown. A good correlation between the guar polymer concentration and the cleanup is observed and quantified. Results from this study show that utilizing this technique can result in an optimum flowback design that maximizes near wellbore conductivity and fracture cleanup for better production.

Direct Analysis of Formation of Asphaltene Scale in Oil Reservoirs

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Session: Industrial Chemistry-Upstream Applications

Asphaltenes are complex, intractable mixtures of low-weight polycyclic aromatic hydrocarbons present in the heavy fraction of crude oil. During the process of oil extraction they are destabilized, and this can result in deposition that causes pipeline blockage and HSE concerns. In the petroleum systems of the Arabian Gulf, asphaltene deposition continues to incur losses of millions of dollars. For the Emirate of Abu Dhabi, where the oil and gas sector accounts for roughly 55% of GDP, a sustainable and long-term approach for mitigation or inhibition strategies are germane to its economic well-being. In the first part of this project, the morphology of asphaltene particles was correlated to the chemical nature of the substrate and asphaltene concentration by using atomic force microscopy. It is demonstrated that uniformly distributed spherical particles form on polar, hydrophilic substrates, whereas irregular islands form on low-polarity, hydrophobic substrates. Additionally, highly concentrated asphaltene solutions result in the development of smooth, thin films, whereas diluted solutions tend to deposit individual nanoparticles. The second part of the project addressed direct quantification of the deposition of asphaltenes by using quartz crystal microbalance (QCM-D). The results provided direct information on the adhesion behavior of asphaltenes, the relative efficacy of different inhibitors, and revealed the best practices for administering inhibitors. Challenges as part of the project as well as new analytical capabilities that facilitate the molecular analysis and highlight the individual complexity of asphaltenes will be discussed. Within broader context, the QCM-D results provide a platform for control of particle morphology, deposition rate, and spatial distribution of asphaltenes, and will lead to the development of smart mitigation strategies.

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Analytical Method in Extracting Sulfur Species from Petroleum Source Rock: Implication for Identifying Sweet Spot in Unconventional Reservoirs

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Abstract Ref Number from the website: ID- 5639
Session: Industrial Chemistry-Upstream Applications

Sulfur species obtained from marine sediments are proven to be invaluable geochemical signatures for reconstructing the deposition condition of a petroleum source rock. Sulfur isotopic signature measured from the sulfur species are useful tracers for the determination of the environmental conditions, and retrieving the original signals of the process, which can help identifying the prolific intervals within the source rock. Conventional analytical methods utilize the bulk sulfur isotope (δ34Sbulk) values measured directly from the whole rock. The δ34Sbulk values could lead to the misinterpretation of the original environmental proxies and unrepresentative isotopic signatures. The aim of this study is to establish a protocol for the extraction of different sulfur species for the purpose of accurately tracing the sulfur isotopic signatures. The protocol was tested on the Paleozoic New Albany Shale (NAS) and the results show that NAS contains four different sulfur species with district sulfur isotopic values. The isotopic signatures from the sequentially extracted sulfur species provide strong and direct proxies for the determination of the paleo-redox condition and the origin of sulfur species in the NAS. The proposed laboratory protocol aided in identifying the zones with potential high hydrocarbon contents and hence optimize exploration and production from the unconventional resources.

Saudi Sand Strengthening with Local Chemicals as Hydraulic Fracturing Proppants

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Abstract Ref Number from the website: ID- 4113
Session: Industrial Chemistry-Upstream Applications

Saudi Arabia has one the most abundant sand resources in the world; however, most proppants used in the hydraulic fracturing jobs are ceramics. Saudi sands have not been used proppants due to the brittle multiple-crystalline nature. To make the brittle Saudi sand good candidate of proppant, chemical coating methods were proposed and improved in this paper.

Saudi sands were treated with local epoxy resins by means of coating. The coated sands were tested by sieve analysis and crushing resistance testing. SEM images were taken for the sand samples before and after crushing. Furthermore, samples with best crushing resistance were selected for long term conductivity test. Saudi sand (high purity silica sand) samples are divided into 3 size distributions: 20/40, 30/50 and 40/70 meshes. Samples from different vendors have been tested and only one of them shows good potential to be used in the fracturing jobs. Before resin coating, pure Saudi sand could stand for only 3,000- 6,000 psi, and after coating with epoxy resin, the product can stand for 8,000-12,000 psi with less than 10% fines. Ratio between resin and sand will affect the strength of final product that higher resin loading shows better results. Multiple coating will tremendously increase the crushing resistance of sand. According to SEM images, two mechanism of crushing resistance improvement were proposed: 1. Smooth surface was observed for Saudi sand after coating with resin, which increase the roundness so as to improve the crushing resistance; 2. Resin coating helps to hold the fines so as not to block the pores between sand grains as well as the formation. In this paper, all the chemicals are manufactured in KSA. This is done to approve the concept that only with local capability, Saudi sand could be also improved and get used in the field operations..

Chemical Approach for Fluid Identification from Oil & Gas Well Exploration

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Session: Industrial Chemistry-Upstream Applications

Well integrity surveillance program is a mechanism applied to Oil and Gas wells to ensure the sound quality and healthiness of all their completion components. Annuli surveys are conducted at regular intervals or in real time for wells that are connected through SCADA to monitor annuli pressures. Data collected during an annuli survey helps identify a problem when it develops and can be used to help determine the causes of problem. During the annuli surveys, unanticipated fluids from different casings were collected for identification. A detailed chemical analysis is required in the laboratory to identify and distinguish this type of fluids.

An unknown fluid was collected from the Tube Casing Annulus of a Gas well formation. The sample was submitted to laboratory for fluid identification and full geochemical analysis. Physical appearance showed milky white turbid liquid with a small oily layer in the surface. The oil was separated using a separatory funnel and the sample was filtered using 0.45micron filter paper. Free flowing with gravity indicated organic contribution, which is confirmed from Sp. gravity test. The sample was further filtered with activated carbon to remove any color. Physical parameters such as pH and conductivity was measured. Since the sample is completely miscible with water, it is assumed to be a mixture of water and an organic solvent with hydrogen bonding. The assumption was also due to severe alcoholic smell from the sample. A full geochemical analysis was performed by eliminating any interferences. HPLC technique was adopted to identify the organic part, which indicated the presence of methanol. Gas chromatographic test was conducted to ensure the methanol content. Moister content was measured using a Karl Fisher Titrator, which indicates 40% moister.

The lab investigation revealed that the submitted sample was a mixture of 40% water and ethanol. Higher anions with minor amount of cations in the sample may be due to contribution from cement degradation or use of any other synthetic chemicals during drilling operation. The production engineers will utilize this lab data for a better root cause analysis of TCA pressure for assuring the well integrity

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR INDUSTRIAL CHEMISTRY PETROLEUM PRODUCTS SESSION

THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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Enhancement of Heavy Oil Production using Viscosity Reducers

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Abstract Ref Number from the website: ID- 5622
Session: Industrial Chemistry- Petroleum Products

Abstract

Chemicals for viscosity reduction can play an important role in enhancing heavy oil production amongst other more commonly used technologies such as crude oil heating by steam, and oil dilution with solvents. The unique features of the viscosity reducer chemicals dissolved in aqueous solutions make it easy to handle and implement in existing water injection infrastructures. These viscosity reducers are composed primarily of a dispersant and an emulsifier. By partitioning into the heavy oil phase, the chemicals weaken the strong interaction among asphaltenes, resulting in a phase inversion from water-in-oil emulsion to oil-in-water emulsion at low water/oil ratio, and facilitating heavy oil mobilization and production.

In this work, thirteen heavy oil reducers were evaluated against a degassed conventional heavy oil. The oil viscosity was 250 mPa.s at 60°C. Evaluation studies included: testing compatibility with high salinity water, measuring interfacial tension (IFT), characterizing rheological properties, and assessing oil displacement using micromodels. Finally, the optimal viscosity reducer was used in a coreflooding displacement test. The coreflooding results were compared against heavy oil production by polymer flooding.

The results show good compatibility of the selected viscosity reducers with a high salinity brine used as the makeup water. The rheological studies demonstrate that a significant heavy oil viscosity reduction was obtained with the introduction of viscosity reducers at a water/oil volume ratio of 30%. Seven viscosity reducers at 2% reduced the heavy oil emulsions viscosities by more than 50%. Oil displacement tests, conducted in micromodels demonstrated, an incremental oil recovery ranging between 10 and 50 % beyond waterflooding. Coreflooding experiments confirmed the optimal viscosity reducer potential. The selected optimal viscosity reducer could increase heavy oil production by 48% of original oil in core (OOIC)—10% OOIC more than that achieved by polymer flooding.

Efficient chemical viscosity reducers provide an economical way to improve heavy oil recovery. They would also reduce the energy consumption associated with recovering, lifting, and pumping heavy oil, i.e. producing heavy oil from the downhole formation to the surface facilities. As such, the application would not only improve well productivity but also reduce operation costs.

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Produced Water: A Review on Characteristics, Challenges and Reuse Opportunities within Oilfield Operations

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Session: Industrial Chemistry- Petroleum Products

Abstract

In oil and gas industry, produced water is considered the single largest volume of byproduct generated during hydrocarbon recovery operations. Produced water is a complex mixture of different organic and inorganic compounds. Due to the increase of activity in petroleum industries across the globe, the generation of produced water has increased all over the world posing a significant issue of environmental concern. Therefore, produced water management and treatment for reuse is now an imperative part of the oil and gas business.

Furthermore, in water-stressed oil-producing countries, the urge to make oilfield produced water be a viable source of reuse has been a growing interest. This review paper aims to highlight the characteristics of produced water, the different treatment options and the possibility of its reuse within the oil and gas main upstream operations. There are various physical, chemical biological methods to treat produced water. However, a comprehensive and deep understanding of each constituent of produced water in relation with the intended reuse application lead to better and more efficient solutions. Based on the latest findings and recently published articles, this paper will discuss in details how produced water can be utilized as a stimulation-based fluid, a water-based for drilling fluid, or as waterflooding application in enhanced oil recovery and what degree of treatment is required for each type of reuse.

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Supporting energy-efficient chemical operations through nano-enabled, enhanced performance

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Session: Industrial Chemistry- Petroleum Products

Abstract

The chemical industry has historically been hard to decarbonize. By using nanoparticle-enabled chemistries, the presented technology signals a step toward lowering the CO2 footprint of the chemical sector in oil and gas production. Specifically, the nano-enabled production chemicals presented here greatly extend the lifetime of chemical treatments (in this case, scale squeezes), which leads to a more energy efficient operation by significantly reducing the volume of chemical required, shortening downtime, reducing required interventions, and increasing economic ultimate recovery.

With this technology, the need for production chemical manufacturing, shipping, and usage by operators for specific applications are reduced by approximately 50-70%. Reducing chemical demand also alleviates the raw materials needed for manufacturing finished products, creating a ripple effect across the supply chain, which supports decarbonization and saves resources. This technology also significantly lowers the CO2 emissions produced during traditional operations by reducing the use of onshore transport vehicles and offshore supply vessels needed to perform squeeze treatments.

Through applying advanced nanotechnology, chemical solutions are generated that have known efficacy, while doubling or tripling the time between required interventions by slowing the release of inhibitor. This technology serves as a template for future developments in other areas of oilfield production chemistry, including asset integrity, microbiology and flow assurance and has the potential for reduction of CO2 emissions and performance improvements in the most prevalent production chemistry issues, which supports more energy-efficient operations.

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Test Methods to Determine the Effect of Diesel Contamination on Gasoline Distillation Properties

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Session: Industrial Chemistry- Petroleum Products

Abstract

Road fuel specifications normally apply at the point of supply to the final customer. The initial determination of fuel quality is usually done at the point of production or blending. Contamination of gasoline by diesel can occur within the transportation and distribution of fuel, and should be controlled by having suitable quality systems in place. Identifying if such contamination has happened, and by how much, is a necessary part of such systems.

An investigation was undertaken to establish the effect of gasoline contamination by diesel on the key specification parameter of distillation. The referee method for the measurement of fuel distillation is ISO 3405 (equivalent to ASTM D86 and IP123) and is the core of the study. To provide further insight an alternative distillation method, ASTM D7345, was also used along with the determination of boiling range by simulated distillation, ASTM D2887, often known as SIMDIS.

For the investigation, gasoline was mixed with known amounts of diesel fuel and tested. Due to diesel being significantly less volatile than gasoline, the end point and residue would be expected to be the most affected by the contamination. The end point by ASTM D86 does not readily detect the presence of low amounts of diesel in the gasoline, whereas the SIMDIS showed a significant response even at very low amounts. SIMDIS methods may not be suitable for quality control purposes, due to the sophisticated equipment required. Conversely, the residue measured at the end of the ASTM D86 test shows a good correlation to the diesel content, and may best represent the concerns that arise from the use of contaminated fuel, whereas SIMDIS testing does not consider residue, and instead simply reports higher boiling components.

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Statistical Quality Control based on ASTM D6299 Using Labware®7 LIMS Platform

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Abstract Ref Number from the website: ID- 5234
Session: Industrial Chemistry- Petroleum Products

Abstract

Statistical techniques to monitor the accuracy of the measuring system is the corner stone for the generation of reliable test data. The range and diversity of the test performed by the lab required an all-encompassing approach that balanced the need versus compliance. This approach has enabled the lab to cover all those analysis that generate quantitative test data well beyond the current scope of ISO17025 certification. While there are various SQC protocols available depending on the application, the gold standard for laboratories is ASTM D6299. The lab team worked extensively to configure LIMS according to the requirements of D6299. There were however exceptions where D6299 was not quite applicable. For those test methods, new SQC protocols were created and configured in-line with the test method requirements and industry best practices.

The additional feature of this SQC program is that it can also calculate Measurement Uncertainty in accordance with ASTM E2554 which will ensure compliance to one of the requirements of ISO17025 Standard. The SQC module was rolled out concurrently with extensive training on the use of this advanced tool to ensure that the users and customers could derive maximum benefits from the system.

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Fossil Fuel an Energy Source: Past, Present, and Future

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Abstract Ref Number from the website: ID- 6198
Session: Industrial Chemistry- Petroleum Products

Abstract

Petroleum Refining has evolved and restructured over the last debates since early 1900s from simple crude distillation operations into increasingly complex operations involving transformation of crude oil into a variety of refined products with specifications that meet the wide array of applications in transportation, power generation, and petrochemical industries. The driving forces for these changes have been different for different periods during the history of refining. This paper will have highlighted the importance of the fossil fuels as a source of energy and the background covering the past to present The following will be discussed & elaborated:

- Evolvement of the refining industry
- Factors Influencing the Future of Refining Industry
- Trends in energy, oil, and petroleum products
- Challenges of the refining industry
- Potential Alternative Fuels for Transportation
- Reasons for the Development of Alternative Fuels
- Challenges Facing Alternatives Fuels Vehicles
- Scenarios for the future

The paper will cover the issue of fuel fuels, needs and impact as source of energy with exclusive summary and conclusion on the current status of fossil fuel and the futurist position as a conventional vs non-conventional non-fossil fuels technologies. The global intention towed this will be also demonstrated.

Saudi Aramco: Company General Use

PROCEEDINGS OF THE GCA-2022 ABSTRACTS FOR POSTER SESSION SESSION

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THE *FIRST* GULF CHEMISTRY ASSOCIATION INTERNATIONAL CONFERENCE AND EXHIBITION (GCA-2022)
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Quantitative Phase Analysis of Sludge Deposits from the Affected Equipment in Refineries and Gas Plants by Use of XRD Data and the Rietveld Method

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Abstract Ref Number: ID- 4313
Session: Advanced Analytical and Laboratory Methodologies

ABSTRACT

The accumulated sludge deposits inside the affected equipment can cause failures. In this paper, the method developed by Sitepu and Al-Ghamdi [Sitepu and Al-Ghamdi (2019) Advances in X-Ray Analysis, 62, 45-67] was extended to accurately and precisely identify the phase identification and composition of the X-ray powder diffraction (XRD) data of the very small quantities of crystalline inorganic materials, which build up in the various equipment at refineries and gas plants. Subsequently, structural, texture, and phase composition of the identified phases were conducted by using the Rietveld method with the generalized spherical harmonics description for preferred orientation correction [Sitepu (2009) Powder Diff., 24, 315-326].

The results revealed that both vanadium oxide (V2O5) and sodium vanadium oxide (NaV2O5) appear in very small quantities of the crystalline inorganic ash deposits. Furthermore, the boiler feed water may contain dissolved oxygen, if the iron oxide corrosion product — in the form of hematite (Fe2O3) — is present in the boiler deposits. Additionally, the presence of metallic copper (in very small quantities in the crystalline inorganic deposits) suggests that there is erosion in the boiler tubes. Therefore special precaution during cleaning operations is required, to prevent copper from plating out. Subsequently, the findings guide the engineers in overcoming problems, by designing chemical cleaning procedures that will not damage the equipment, and thus avoid future equipment failure.

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Evaluation of Organically Crosslinked Polymer Gels for Conformance Application in Harsh Reservoir Conditions

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Abstract Ref Number: ID- 4322

Session: Industrial Chemistry -- Enhanced/Improved Oil Recovery

ABSTRACT

Polymer gels have been applied as fluid diverting or blocking agent to improve oil displacement efficiency in petroleum industry. Heterogeneity is often observed in many oil reservoirs, which severely hinders the efficient sweep of oil. Gel-based conformance control is a potential technique to ensure fluids optimally contact the remaining oil. However, in-depth conformance control in high temperature reservoirs is still a challenge, due to the difficulties to achieve longer gelation time and thermal stability.

In this study, we evaluate organically crosslinked polymer gels for in-depth conformance improvement application in high salinity and high temperature reservoirs. Polymer and gelant solutions are prepared anaerobically in a glove box. The gelant solutions are then sealed in glass tubes and aged at high temperature. The flowability of the gel samples are periodically observed for evaluating the gel strength variation, determining the gelation time, and assessing long-term thermal stability.

Three polyacrylamide polymers were used in this study, which were crosslinked by three organic crosslinkers, polyethyleneimine (PEI), hexamethylenetetramine (HMTA) and hydroquinone, and HMTA and resorcinol. The effects on gelation performance of temperature, polymer molecular weight, polymer and crosslinker concentrations, and brine salinity were investigated. Results showed that the gelation time of the studied gel systems reached five to seven days at 95°C, with sufficient gel strength and long-term stability. Temperature had significant impact on gelation time, and lower temperature helped to achieve longer gelation time. Gels with low molecular weight polymers showed longer gelation time and longer thermal stability. Gelation time became longer when decreasing either polymer or crosslinker concentrations, but there were lower concentration limits to form gel. The studied gels had a wide range of tolerance to brine salinity. The results in this work demonstrate the potential of the studied organically crosslinked gels for in-depth conformance application at harsh reservoir conditions.

Enhancing Foam Stability Through A Combination of Surfactant and Nanoparticles

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Session: Materials -- Functional Nano-Materials and Nanotechnology

ABSTRACT

Gas injection is amongst the most commonly used EOR methods, however it is subject to poor macroscopic sweep efficiency due to the higher mobility and lower density of gas compared to reservoir fluids. Foamed-gas injection can regulate the mobility of gas, increasing the apparent viscosity and reducing the gas's relative permeability. Nevertheless, the poor stability of foam at harsh reservoir conditions is a major limitation that hinders the effectiveness of the foam flood. A combination of surfactant and nanoparticles (NPs) provides a novel solution to these challenges.

This study evaluates the role of NPs on enhancing foam stability. Static and dynamic laboratory tests were conducted to capture the foam stability and strength in porous media for different surfactants combined with surface modified silica NPs. The static foam stability was determined by measuring the foam half-life over time. The dynamic foam stability was determined through the mobility reduction factor using micromodel apparatus.

The results from the experiments show that the use of surfactant combined with NPs enhances the stability and strength of the generated foam. The foam static tests show that the mixture of NPs and surfactants produces foams with smaller bubbles and longer half-life when compared to those in the absence of NPs. The results also demonstrate that the concentration of surfactant and NPs is a crucial parameter. In porous media, the addition of NPs results in larger pressure drops across the micromodel chip when compared to using surfactant solution alone. The results also reveal that the generation of NPs flocs is the main mechanism of foam stabilization enhancement

This work shows that using NPs at carefully selected concentrations in combination with surfactants can improve the foam static and dynamic stability in porous media, effectively improving the sweep efficiency of gas compared to the typical application of using surfactants alone.

Thickened-CO2 for Waterless Fracturing Applications

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Session: Carbon Capture and its Applications

ABSTRACT

Hydraulic fracturing technology has grown popular with the rapidly increasing development of tight conventional and unconventional reservoirs. However, a major concern with this technique is the use of large amounts of water in these treatments. The use of water causes many issues in the formation and limits the amount that can be saved for future generations. We are proposing a CO2 fracturing technology that eliminates the need for water in hydraulic fracturing.

Water-based fracturing fluids can cause a variety of issues during and after the fracturing treatment. Hydraulic fracturing treatments consume at least 200,000 gal of water per stage. The pumped water must include clay stabilizers to deal with the clay sensitive and clay rich formations such as shale formations. In addition, when the pumped water is incompatible with the formation water it will cause precipitation of inorganic scale which will increase near wellbore skin. Only a mere 10-30% of pumped water flows back after the treatment, with the rest attached to clays, or in the pores due to high capillary pressures. Water-based fluids also causes alterations to relative permeability and blocks the gas flow creating ‘water blockage’ cases. Liquid holdup can also arise due to the use of water in many gas wells. At the end of the treatment water still causes issues related to disposal and separation prior to diverting it to the plant.

Our idea will help ease off the pressure on freshwater resources significantly. The main obstacle in the industry to developing such a technology has been the low viscosity of liquid CO2. However, we have identified an environmentally friendly thickening agent that is soluble in CO2 at practical conditions. Waterless fracturing with liquid CO2 is expected to efficiently stimulate the reservoir at a lower operational cost without causing damage to the reservoir, while reducing emissions and protecting our environment.

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Functionalized Nano-Platelet Based Novel Resin Emulsion Nanocomposites for Material Strength Enhancement in Proppant Fracturing Applications

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Session: Industrial Chemistry -- Polymer and Nano-Composites

ABSTRACT

In a hydraulic fracturing operation, a fracturing fluid is pumped at high pressures along with proppant to fracture the formation for producing hydrocarbons. The primary aim of proppants is to prevent the fracture from collapsing under overburden stress of the formation. The permeability and conductivity of a propped fracture can be affected due to proppant crushing and overall strength depletion of the proppants. Resin coated proppants are widely used in hydraulic fracturing applications to increase the strength of proppant material to withstand closure stresses and to mitigate any proppant flowback. In this paper we showcase the development of nano-platelet based nanocomposites that enhance the proppant material properties. The structure property relationship of these novel nanocomposite materials and its importance in choosing the type of fillers in composites is also discussed.

The development of novel polymer based nanocomposites comprising of emulsified resin and nano-platelet shaped filler materials is discussed. The resins used for proppant coating are introduced as a water external emulsion, thus making them compatible with the aqueous fracturing fluids. We show that by using a these type of emulsion system as proppant coating material we could introduce this system on the fly, along with the fracturing fluid without facing any incompatibility issues between the hydrophobic resin and the aqueous fracturing fluid. We further show that by using platelet shaped filler materials dispersed within the emulsified resin we could tremendously enhance the overall material properties of the proppants.

The nanocomposites are developed in-situ due to delamination of the individual nano-platelets into the emulsified resin matrix. A study of different conditions under which optimum material property enhancement can be achieved is discussed. Various chemical modifications of the nano-platelets required for enhanced compatibility with the emulsified resin that would lead to better thermo-mechanical properties are demonstrated. We showcase the microstructural evaluation of the nanocomposites and its effect on thermal and mechanical properties of the proppant coating material.

Novelty of this paper is the development of new nano-platelet based proppant coating materials that lead to tremendous material property enhancement. The operational advantage of on-the-fly deployment of the proppant coating material along with fracturing fluid due to enhanced compatibility is also presented.

Saudi Aramco: Company General Use

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Evaluation of Alkalinity Transfer into Condensed Brines in Oilfield Wells

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Session: Industrial Chemistry -- Petroleum Products

ABSTRACT

Oilfield operators in the Bakken have experienced unanticipated calcium carbonate plugging in surface lines. While easily addressed through use of HCl or replacement of plugged piping, ChampionX worked to identify the root cause of these surprise deposit.

Since the calcium carbonate deposits were occurring at a commingle point, ChampionX collected samples of condensed brine from the casing production stream to compared with the produced brine from the production tubing stream. While Bakken production brine is typically low in bicarbonate (<400 mg/L) and high in calcium (>10,000 mg/L), the condensed brine contained as much as 30,000 mg/L bicarbonate. The bicarbonate content of the condensed brine was not anticipated, and so the source of the high bicarbonate was evaluated.

Unexpectedly, it was discovered that the high bicarbonate content in the condensed brine could be replicated through a simple distillation experiment. This unexpected high bicarbonate generation in condensed brine required additional studies to better understand this unique situation. In addition to working to understand how the alkalinity could transfer into condensed brine, ChampionX evaluated whether a similar alkalinity transfer could occur with produced brines from other production basins.

The identification of this apparent alkalinity transfer into condensed brines in oilfield wells has potential implications for operators who commingle production streams off the wellhead after producing gas up the annulus and fluids up the production tubing. Identification of this phenomena will allow operators to understand the root cause of such surface plugging and take appropriate measures to avoid its impacts.

Advancement in the Analysis of Aromatic Hydrocarbons and Sulfur Heterocycles in Petroleum Samples using Liquid Chromatography and FT-ICR MS

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Session: Advanced Analytical and Laboratory Methodologies

ABSTRACT

Crude oil remains a key source of energy to meet the continued demand for transportation fuels, in addition to a substantial growth as feedstock for petrochemicals. With the progress towards cleaner transportation fuels to address environmental issues, a successful characterization of aromatic hydrocarbons and sulfur heterocycles in petroleum streams remains inevitable. This knowledge helps in choosing the right catalysts and process conditions for the efficient utilization of non-renewable resource to produce cleaner gasoline, jet fuel, diesel, and marine fuels. One of the key steps in such characterization work is the determination of ring-number and average alkyl chain length of aromatic compounds. The number of rings plays a decisive role in different catalytic reactions in refining processes. Simultaneously, position and length of alkyl groups greatly influence the efficiency of catalytic reactions.

For successful characterization of aromatic compounds, we employed liquid chromatography methods for the separation of petroleum samples and ultrahigh resolution mass spectrometry for the molecular level characterization of nonpolar hydrocarbons and sulfur heterocycles. In liquid chromatography, two separation modes were employed: (1) normal phase chromatography for the separation according to ring number and (2) size exclusion chromatography for the separation according to alkyl chain length of aromatic compounds. The ultrahigh resolution mass spectrometry measures the accurate ring number and alkyl chain length of the aromatic compounds. The presentation will cover the development of analytical methods using liquid chromatography and mass spectrometry, its application to petroleum samples, advancement in the analysis in comparison to reported literature and its limitations for extremely complex sample such as crude oil mixture.

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Advanced X-ray analytical techniques to support the development of innovative materials

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Session: Advanced Analytical and Laboratory Methodologies

ABSTRACT

The development of innovative materials is a concerted action between several disciplines. Together with the chemical effort, physical and analytical ones are necessary in order to determine the characteristics and the properties of the newly synthesized species.X-ray based techniques can be ideal tools for a quick and accurate analysis of several aspects of a material. Modern X-ray diffraction techniques, for instance, are able to provide quantitative information about chemical purity and atomic arrangement (structure), as well as information on the microstructure such as shape and size distribution of the crystallites, type and quantity of lattice defects, orientation of the crystallites. When exploited at large scale facilities (e.g. synchrotrons, neutron sources, X-ray Free Electron Lasers), diffraction can also help in fast screening (tens of thousands specimens handled and analyzed automatically), for in situ and in operando analyses (e.g. during synthesis, transformation, in operation), to obtain volumetric phase information (diffraction tomography) or provide further unexpected data (e.g. activation energies, short and long range order). The simultaneous availability of complementary techniques (e.g. Raman or FTIR spectroscopy), further widen the range of applications.These advanced tools, with or without the support of Artificial Intelligence, can improve the capability of the chemist for faster development of a material possessing new or improved properties.

Some basic information and practical application cases will be illustrated and discussed.

Iron Sulfide Scale in sour wells, from causes to remediation

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Session: Industrial Chemistry -- Petroleum Products

ABSTRACT

Deposition of different types of inorganic scales on the inner walls of oil gas reservoir is one of the persistent challenges that interferes with field operations. The analytical investigations of these deposited minerals showed significant variations with respect to composition and structure within the collected samples. However, the major contribution is found to be from different minerals containing ferrous cation such as (pyrrhotite, troilite, mackinawite, pyrite, marcasite and greigite) or ferric cation (hematite, maghemite, akaganeite, goethite and lepidocrocite).

The descaling of these minerals often involves two methodologies: (1) the chemical dissolution involving strong inorganic acids and (2) mechanical removal. The former usually results in corrosion of the steel pipelines and later very laborious in nature. Moreover, FeS being hydrophobic on surface gets coated with oil phase which minimizes the contact of aqueous acids with deposited mineral. The other methods include addition of scale inhibitors depending on the chemical nature of scale and oil well operating conditions. However, most of these inhibitors are unstable at temperature 140 oC or above

The overall objective of this paper project is to characterize the chemical composition, structural architecture and morphology of the deposited scalants followed by designed synthesis and characterization of new anticipants this research work will focus on the following specific materials design goals

A thorough characterization of the chemical composition and structure of scalants to better understand the chemistry or physical structure using different X-rays, spectroscopic and microscopic based analytical tools was used. Surface engineering/functionalization to ensure various interfacial compatibilities for the targeted applications as well as syntheses of various antiscalants upon finding a promising candidate at a given stage of the research project.

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Novel systematic approach to Oil-field carbonate scale dissolution and characterization

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Session: Advanced Analytical and Laboratory Methodologies

ABSTRACT

Scale formation in the wellbore and pipelines during upstream processes cause production upset and decline in revenue. Hence treatment and removal of oil field scales are important for avoiding production depreciation. Scale varies in chemical composition, being composed of layers of scale adhering to the inside of tubing and deposited during the well lifecycle. Identifying the location and composition of the scale deposit is the first step in designing a cost effective remediation program. Scale removal could be mechanical or chemical. Scale removal technique must be quick, non-damaging to the wellbore, tubing or formation environment, and effective at preventing re-precipitation. There have been many significant advances in scale control and remediation in recent years. The improvement in placement technology, reservoir chemistry and intelligent fluids furnish more cost effective options for chemical scale inhibition or removal in downhole tools. The purpose of the present study was to analyze the scale composition and then develop and recommend a solution to effectively remove specific oil field scale from downhole tools. In this study, scale samples were collected from downhole tools and determined the compositional analysis of scale samples to characterize both crystalline and non-crystalline compounds. Composition of scale samples has been determined by X-ray Diffractometer (XRD), X-ray Flourescence (XRF), inductively coupled plasma atomic emission spectrometry (ICP-AES) and acid solubility to determine a more accurate scale composition analysis. XRD and XRF results showed that scale composition is mostly carbonate. Based on scale composition, treatment fluids were designed to evaluate scale dissolution capability and also studied the corrosivity of scale dissolver in the presence of various corrosion inhibitors.

Effective Adsorption Heavy Metals from wastewater by using polyamide - graphene (PAG)

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Session: Materials for Environment and Wastewater Purification

ABSTRACT

Effective Adsorption Heavy Metals from wastewater by using polyamide - graphene (PAG)

Since discovery graphene ,it is became a rising star in the field of nanomaterials. In the few last year's, graphene attracted the attention of the materials scientists, because of its distinctive properties that have no analogy and have a role in changing the future. The graphene has interesting properties such as high electrical and thermal conductivities. Furthermore, its cost of production, the abundance of raw source materials preludes it to be used in every aspect of modern life. Although, these wide ranges of potentials applications. Graphene was modified with polyamide by using a facile interfacial polymerization method to obtain an effective composite. The produced polyamide-graphene (PAG) was characterized by Fourier transform infrared spectroscopy (FTIR), Scanning Electron microscopy (SEM) equipped with Energy-Dispersive X-ray spectroscopy (EDX), Thermogravimetric analyzer (TGA), and Brunauer–Emmett–Teller (BET) analysis methods. The adsorption efficiency of the adsorbent for the removal of heavy metals such as (Cd, Cr, Pb, Hg) was evaluated under the effects of concentration, temperature, contact time, medium pH, and re-usability. The results of the study showed very good adsorption performance and high regeneration. And the concentration of minerals decreases in the solution when using graphene polyamide by 99% from 5 to 0.1 mg/L. All the results were considered in designing a filter that is filled with the compound and passing the eluent solution that contains the minerals or metal ions. The eluate was collected, and the analysis results showed the water free of heavy metals indicating the high efficiency of the compound.

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Inhibition of Concentrated HCl Acid Solutions Used in Matrix Acidizing Treatments Using Synthesized Amine-based Corrosion Inhibitors

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Session: Industrial Chemistry -- Enhanced/Improved Oil Recovery

ABSTRACT

Mono and diamine compounds were synthesized from dodecylamine and 1,12-dodacanediamine, and evaluated as acid corrosion inhibitors for coiled tubing steel. The inhibition behavior of these compounds in concentrated HCl acid was examined using gravimetric method. Weight loss tests were conducted in 28 wt% HCl acid at 70oC for 2 hours. The effect of intensifier on inhibited concentrated HCl acid solutions was investigated.

The results showed that both mono and diamine inhibitors exhibited a good protection efficiency for coiled tubing steel in 28 wt% HCl acid. However, monoamine compounds showed better performance. Addition of an intensifier was effective to enhance protection efficiency for both amine moiety compounds where more than 99% protection was obtained for some inhibitors. The effect of intensifier concentration on inhibition efficiency is also addressed in this paper. The results obtained are very promising and suggest that some of examined corrosion inhibitors have a good potential to inhibit acids used in stimulation treatments of oil/gas wells.

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From Lab-to-Field: Successful Deployment of a Novel Retarded Acid System for Deep-Reservoir Stimulation of Carbonate Reservoirs

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Abstract Ref Number: ID- 4983
Session: Industrial Chemistry -- Enhanced/Improved Oil Recovery

ABSTRACT

The oil and gas industry relies on the use of chemical methods for well stimulation of carbonate-rich formations, in particular hydrochloric acid (HCl). It remains a challenge however to successfully enhance the fracture half-length in acid fracturing operations using only HCl. Among various methods and retarded acid alternatives, emulsification of HCl-in-diesel remains the most widely used. This approach however poses significant field limitations that include high friction pressures, limited thermal stability and complex mixing procedures. As a result, there exists a need for an alternative retarded acid system that addresses these shortcomings, while preserving the advantages such as high dissolving power.

Accordingly, a novel engineered hybrid acid system coined LVAS-1 was developed and prepared by blending a strong mineral acid with a suitable strong organic acid. In order to achieve the requisite kinetic profile, the amount of water in the formulation was fine-tuned as a strategy to slow down the dissociation of the acid. Most notably, this acid system reduces operational complexity at the wellsite, enables pumping at high rates and exhibits superior retardation properties. The technology was recently field tested in a high temperature/high pressure carbonate reservoir in the Middle East. Single-stage acid fracturing treatments were performed in two individual conventional gas wells and both responded very well to the treatment. Post–treatment analysis was conducted to evaluate the performance of LVAS-1 and benchmark it to acid systems previously tested in the field. This includes pressure transient analysis, post–fracturing flow back and friction pressure calculations. Pressure measurements relied on the installation of downhole gauges for friction calculations and Pressure Build-up analysis.

This poster describes a success story, i.e. from laboratory-to-field scale, in the development and utilization of new retarded acid system, while it highlights design parameters as well as highlights the advantages and limitations over the conventional retarded acid system.

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Enhance Productivity for Shale Gas Reservoirs: Increasing SRV Using Thermochemical Treatment

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Session: Industrial Chemistry -- Enhanced/Improved Oil Recovery

ABSTRACT

Enhance Productivity for Shale Gas Reservoirs: Increasing SRV Using Thermochemical Treatment

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Abstract

In shale reservoirs, the gas productivity is severely reduced due to the formation tightness. The extreme low permeability of shale formations can result in reducing the gas flow into the borehole, and consequently the gas production can be significantly reduced. This paper presents an effective technique for enhancing the gas productivity for shale gas reservoirs using thermochemical fluids. The used chemicals can generate heat and pressure in-situ and improve the flow condition by creating micro- factures in the shale rocks. Experimental measurements and analytical calculations were carried out to investigate the enhancement in gas productivity for shale samples due to the injection of thermochemical fluids.

Core flooding experiments and rate transient analysis (RTA) were conducted as well as nuclear magnetic resonance (NMR) measurements. Tight core samples from eagle ford formation were used in the flooding experiments. The improvement in gas productivity due to thermochemical injection was evaluated using rate transient analysis. The profiles of pressure-drop and gas flow-rate were used to estimate the gas productivity before and after the chemical treatment. NMR measurements were used to study the changes in the

pore network due to thermochemical stimulation. The T2 signal distribution was obtained before and after the chemical injection. Furthermore, analytical calculations were performed to estimate the enhancement ingas productivity due to the thermochemical treatment. The increase in absolute open flow (AOF) and the productivity index (PI) due to the chemical treatment were determined.

Results showed that treating shale rocks with thermochemical fluids can enhance the gas productivity by62% and reduce the capillary pressure by more than 45%. Also, the absolute open flow can be increased four times due to the thermochemical injection into shale reservoirs. The generated heat and pressure due to thermochemical treatment can induce permanent alterations in the shale matrix and then improve the hydrocarbon flow for long term. NMR measurements, before and after the treatment, confirm the creation of tiny fractures during the chemical injection. The novelty of this work is that an effective treatment is presented to enhance the gas productivity for shale formations. Ultimately, this study will be very useful for treating the shale reservoirs with thermochemical fluids to improve the gas productivity, and consequently enhance the total gas production from shale reservoirs.

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IPTC-19603-Abstract

Keywords: Shale reservoirs, gas productivity, effective treatment, thermochemical injection, rate transient analysis

Big Data Role in Determination Arabian Gulf Seawater Quality

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Session: Fourth Industrial Revolution (IR 4.0) -- Big Data

ABSTRACT

In this paper, a study was conducted to assess the Total Coliform bacteria and hydrocarbons contamination levels in correlation with the other physicochemical properties of the Arabian Seawater. Total of 21 water samples were collected, with 7 samples from each zone A, B & D at Qurryah Sea Water Plant, at an interval of one month between each batch. Zone A (Intake Channel), Zone B (Discharge), Zone D (Discharge) at Qurryah Sea Water Treatment Plant, starting from January to July 2019. The following instruments have been utilized to perform the analyses required for this study: Colilert from IDEXX per Standard Methods: EPA 9223B Enzyme substrate assay for quantify both the total coliform and Escherichia coli (e-Coli) bacteria, Eracheck eco (Mid-IR Laser Spectroscopy) from eralytics to measure the Oil & Grease and Total Petroleum Hydrocarbons concentrations per ASTM D7678-17, SPE-DEX ® 5000 Automated Extraction System from Horizon technology to extract the hydrocarbons from the seawater samples used to minimize human errors and for consistent extraction, Mettler Toledo T90 Auto-Titrator for carrying out the Chloride analysis, and ORION model 162 for measuring the conductivity of the Qurryah seawater samples. Zone D (Discharge) showed the highest Total Coliform concentration (Max.: >1600 MPN/100 mL), while Zone A (Intake Channel) was the second highest of the Total Coliform concentration (Max.: 866 MPN/100 mL). QB (discharge) showed the lowest contamination of the Total Coliform with (Max.: 225 MPN/100 mL). There was a clear association between the Total Coliform index and Oil & Grease and Total Phosphate. The power of data science and algorithms was exploited to predict the seawater quality and create the ‘fingerprint’ of the shoreline of the Qurryah Sea Water together with the two discharge-points (Zone B & D) at Qurryah

Sea Water Treatment Plant. The study concludes that the Arabian Gulf is highly vulnerable for the fecal and coliform pollutions especially if we know that the Arabian Gulf Seawater is less buffered compared to the others nationwide. Also, algorithms such as 'K-means' for clustering and 'KNN' for data modeling have successfully demonstrated the profile of the Arabian Gulf Seawater where each Zone set apart from other by computing the parameters per each. This technique can help proponent in investigating the problems and easily find the source of water. Lastly, this technique can also be applied to other industrial areas of interest to find out the source of fluids based on the collected data parameters.

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Well-defined Linear Amphiphilic Diblock Copolymers of 2-Ethyl-2-Oxazoline and Vinylidene Fluoride; Synthesis and Characterization

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Session: Industrial Chemistry -- Polymer and Nano-Composites

ABSTRACT

Linear Amphiphilic Diblock Copolymers of 2-Ethyl-2-Oxazoline and Vinylidene Fluoride; Synthesis and Characterization

Well-defined linear diblock copolymers with a hydrophobic fluoropolymer poly(vinylidene fluoride), PVDF and a hydrophilic poly (2-Ethyl-2-Oxazoline), PEtOx block, were successfully synthesized by combination of cationic ring-opening polymerization (LCROP) and reversible addition-fragmentation chain transfer (RAFT) polymerization techniques.

PEtOx was synthesized by LCROP of 2-ethyl-2-oxazoline (EtOx) monomer followed by two post-polymerization reactions, esterification, and nucleophilic substitution to introduce at the chain end the necessary RAFT agent, i.e., xanthate for the sequential RAFT polymerization of fluorinated monomer, i.e., VDF and afford the PEtOx-b-PVDF diblock copolymers.

The success of the synthesis of the macrotransfer agent and final diblock copolymers was confirmed by Proton Nuclear Magnetic Resonance Spectroscopy (1H-NMR) and Fourier Transform Infrared Spectroscopy (FT-IR). The number-average molecular weight (Mn) and the polydispersity index (Đ) of the copolymers, determined by Size Exclusion Chromatography (SEC), were 10.5–64 k and ≈1.2, respectively. The thermal properties, including glass transition (Tg), melting (Tm), and crystallization temperatures (Tc), were studied by Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry

(DSC). The self-assembly of the amphiphilic copolymers in water/DMF was evaluated using dynamic light scattering (DLS) and the polymorphism by X-Ray Diffraction (XRD).

The synthesized amphiphilic diblock copolymer combines both properties of PEtOx and PVDF, and thus render them a good candidate for biological and industrial applications.

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Acid Corrosion Inhibition Using Graphene Oxide Based Nanomaterial

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Abstract Ref Number: ID- 6112

Session: Materials -- Functional Nano-Materials and Nanotechnology

ABSTRACT

This work details the preparation of graphene oxide based nanomaterials from graphite and also investigate their performance as corrosion inhibitors. The synthesized materials were characterized using Raman spectroscopy, Fourier-transform infrared spectroscopy, transmission electron microscopy, and thermogravimetric analysis techniques. Temperature and concentration effects on inhibitors performance were also looked into.

The inhibitory efficiency increased with concentration at room temperature, reaching about 84% at a concentration of 5 ppm for the dodecane modified graphene oxide. The inhibitors primarily function as cathodic inhibitors. The Langmuir adsorption theory was found to be followed by the studied compound. The dodecane modified graphene oxide molecules adsorbed on the steel surface to create a protective layer that insulated the steel surface from the aggressive acid assault after the immersion time in the inhibited solutions. DFT calculations were utilized to determine the relative stability of functionalized graphene against graphene only and to learn more about the inhibitor molecules' interactions with the steel surface.

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Aromatic Compounds Variations with Thermal Maturity in Crude Oils

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Session: Industrial Chemistry -- Exploration/Geochemistry

ABSTRACT

Ranking crude oils based on the effect of thermal maturation is vital for the analysis of petroleum systems as well as basin modelling. For this reason, biomarkers are studied to assess the maturity of the crude. However, due to their thermal instability, maturity indicators fail to cover the whole oil and gas windows. Therefore, in this study, we have investigated the application of aromatic-based maturity indicators on a series of varying maturity crude oils. Five oil samples were collected from various depths, fractionated using solid-phase-extraction with silica-gel, and the aromatic fractions were isolated, then analyzed using gas chromatography equipped with a triple-quadrupole mass spectrometer. Aromatic compounds including Naphthalene, Phenanthrene, and Dibenzothiophene were targeted for this analysis. The maturity ratios were calculated based on the peak areas of the targeted aromatic compounds. Several Naphthalene and Dibenzothiophene-based maturity ratios showed a correlation with increasing maturity and with conventional biomarker maturity indicators such as triaromatic steroids (TAS). These new ratios showed a systematic change from low-maturity oil with an API of 24 to high-maturity oil with an API of 41.6. The maturity of the crude oil can help in the calibration of basin models as well as in understanding hydrocarbon migration paths in sedimentary basins. The existing biomarker-maturity ratios are limited to a narrowed maturity window. Therefore, the present work focuses on aromatic-based maturity ratios that can optimize the crude oils' maturity ranking in higher maturity crude oils where conventional biomarkers fail to work.

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Evaluation of Cold Flow Improver Additive of Riyadh Winter Diesel

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Session: Industrial Chemistry -- Petroleum Products

ABSTRACT

During unseasonably cold weather, diesel fuel is prone to waxing at temperatures below its cloud point due to solid wax crystals formed by straight chain n-paraffins grow within the fuel. As the temperature is lowered further these crystals increase in size, agglomerate and eventually separate from the bulk fuel giving it a cloudy appearance. This can cause operating difficulties, such as blocking fuel system filters and lines resulting in poor starts, engine hesitation, stalling and even engine damage in both mobile and stationary applications.

To address this problem, Saudi Aramco makes available winter diesel fuel with cold flow properties tailored to avoid the wax separation issue. This can be achieved by either blending kerosene or cold flow improver additive (also known as wax crystal modifier additive) into the diesel fuel before the product leaves the refinery.

Saudi Aramco's Research and Development Centre (R&DC) has systematically evaluated the use of fuel additives both in refining and distribution system. The key objective of this study was to identify suitable additives that can improve the cold flow properties of Riyadh Refinery's winter diesel fuel.

The evaluation process conducted in two parts. In Part 1, five (5) foremost diesel fuel cold flow improver additives were identified based on a thorough literature and market search as well as on subject matter expert recommendations. During Part 2, the performance of the selected cold flow improver additives was evaluated based on the Cold Filter Plugging Point (CFPP) response for different treating rates of the cold flow improver additive by applying the ASTM D6371 test method over a retained sample of winter diesel fuel from Riyadh Refinery.

The overall findings on the additive performance were summarized into a ranking "score" and can poses valuable information for operation crews and process engineers, as well as, industrial hygiene and asset management teams.

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Enhancement of Tetralin Hydrogenation over Supported Nickel Catalysts

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Abstract Ref Number: ID- 4109

Session: Catalysis -- Catalysts-Based Nanotechnology

ABSTRACT

Hydrogenation and reduction of poly-aromatic compounds to enhance diesel and Jet fuels has received considerable attention recently to comply with global fuel specification and overcome future limitations. The characteristic properties of the current transportation fuels show high content of poly-aromatic compounds (mostly di-aromatic compounds) which reduces the fuel efficiency. In the literature, naphthalene and tetralin have been selected as a representative models for poly-aromatic compounds. The hydrogenation of naphthalene was studied intensively in the literature. However, less attention has been paid to its hydrogenated product (i.e tetralin (1,2,3,4-tetrahydronaphthalene)). It has been reported that hydrogenating tetralin is much more difficult than naphthalene. In this project an investigation was carried out to study the feasibility of using nickel catalytic systems synthesized by different methodologies and metal precursors for the hydrogenation of tetralin. The study entailed characterizing the synthesized catalyst using BET, AAS, TGA/MS, and XRD before and after the reaction. The catalytic activities of the synthesized catalysts were determined using a continuous down flow fixed bed reactor under different reaction conditions. The catalytic activity test results revealed that the performance of the synthesized in-house catalyst exceeded the activity achieved by literature nickel catalysts at lower reaction conditions. Different activities were recorded for different reaction parameters. A notable difference was observed in the trans/cis ratio of the products using catalysts prepared with different nickel precursors. The spent catalysts were post-characterized and showed significant amount of carbon laydown.

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Determination of low-level of Arsenic in solid sulfur by hybride generationatomic absorption spectroscopy (HGAAS)

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Session: Materials for Environment and Wastewater Purification

ABSTRACT

DETERMINATION OF LOW-LEVEL OF ARSENIC IN SOLID SULFUR BY HYDRIDE GENERATION ATOMIC ABSORPTION SPECTROSCOPY (HGAAS)

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Abstract

Arsenic (As) is a toxic trace element that can be found in many sources, including crude oil which is then transformed and refined into useful products, such as LPG, gasoline, diesel, heavier distillate and solid sulfur and that is a byproduct for removing sulfur-containing contaminants from natural gas and petroleum cuts, prior to be in demand. Arsenic can be released from these products to environment through the production of hydrocarbons and chemicals, storage, transportation and use, causing serious health impact on human and pollution effect on environment, thus, they are considered as undesirable constituents in the product. Although, there are many analytical methods for Arsenic determination in waste water, petroleum and soil samples, i.e. Graphite furnace atomic absorption spectrometry (GFAAS) (EPA 7010). Determination of arsenic in heavy petroleum fractions by GFAAS (UOP986) (assisted by sample mineralization in a microwave oven), Arsenic in Naphtha and Gasoline by HGAAS (UOP946), Trace Arsenic in Liquid Organics and Heavy Petroleum Fractions by ICP-MS (UOP992), yet, there is no approved test method covers the determination of Arsenic in solid Sulfur has been published, taking into consideration that (YASREF) produces 1,200 tpd of pure solid sulfur, plus the customers' requirements, all that were the engine to develop this test

method on the highest possible level of accuracy. The extraction and determination of Arsenic in solid Sulfur is challenging due to three reasons, first, the low-level of concentrations of its compounds in such product, second, the possibility of loss during treatment of sample, last, the Arsenic species are very sensitive to air, exposure can cause changes in species over time. As demonstrated here, a HGAAS-based method was developed by taking advantage of hydride-forming property of Arsenic to quantitatively determine its concentration in solid Sulfur. Commercial use of the solid sulfur is the production of sulfuric acid for sulfate and phosphate fertilizers, matches, insecticides and fungicides.

In this study, a sensitive method was examined and developed for the determination of Arsenic concentrations in solid Sulfur by Hydride Generation Atomic Absorption Spectroscopy (HGAAS). A weighed sample is mixed with Magnesium Oxide and Sodium Carbonate and ignitied at 750oC. Mixture is then digested with hydrochloric acid, and reduced with Potassium Iodide. The gaseous hydride of Arsenic is generated from the appropriate oxidation state using Sodium borohydride as reducing agent. The method was validated by spiking with Sodium Arsenite (Na_3AsO_3); recovery of 80% was obtained at 20 µg/L-1 level. Limits of detection (LOD) and limits of quantitation (LOQ) were calculated to be 0.9 and 1.0 µg/L-1 , respectively.

As conclusion, This study has demonstrated the ability of efficient extraction, dissolution, reduction and determination of Arsenic in solid Sulfur providing an alternative method to ICP-OES instrument, in addition to the advantage of HGAAS that requires smaller volume of sample and high accuracy of results obtained at part per billion range of concentrations

In this study, a sensitive method was examined and developed for the determination of Arsenic concentrations in solid Sulfur by Hydride Generation Atomic Absorption Spectroscopy (HGAAS). A weighed sample is mixed with Magnesium Oxide and Sodium Carbonate and ignited at 750oC. Mixture is then digested with hydrochloric acid, and reduced with Potassium Iodide. The gaseous hydride of Arsenic is generated from the appropriate oxidation state using Sodium borohydride as reducing agent. The method was validated by spiking with Sodium Arsenite (Na_3AsO_3); recovery of 80% was obtained at 20 µg/L-1 level. Limits of detection (LOD) and limits of quantitation (LOQ) were calculated to be 0.9 and 1.0 µg/L-1 , respectively

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Continuous fixed bed CO2 capture using activated carbon: breakthrough, equilibrium, efficiency and mass transfer zone

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Session: Carbon Capture and its Applications

ABSTRACT

The post-combustion CO2 emissions are the result of increased worldwide energy demand and there is pressing need to regulate the CO2 level in environment before rigorous and lasting damage to climate system is done. The CO2 separation from feed consisting of CO2 and N2 employing activated carbon as an adsorbent has been explored in a continuous fixed bed unit. The FESEM and Brunauer-Emmett-Teller analyzer have been used to examine textural and structural properties, respectively. The breakthrough curves have been produced as a function of temperature and feed flows. The reliance of CO2 capture capacity on temperature, feed rate and adsorbate partial pressure has been investigated. The breakthrough time relies strongly on temperature and feed rate. The performance of adsorbent has been judged in terms of breakthrough and saturation periods, column efficiency, usable bed height, length of mass trasnfer zone and capacity utilization factor. The good CO2 uptake of 0.98 mmol/g was evaluated at 298 K with feed flow of 5 slpm and Co= 5%. The practicability of porous carbon for CO2 capture is also confirmed by acceptable utilization factor of 0.92 at 298 K. The commercial adsorption of CO2 owing to high CO2 uptake and excellent adsoprtion characteristics may be carried out utilizing the activated carbon.

Mesoporous black TiO 2 supported mono- and bimetallic Au-Pd Nanoclusters for efficient photocatalytic H 2 generation

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Abstract Ref Number: ID- 5364

Session: Catalysis -- Photo-Catalysis

ABSTRACT

Mesoporous black TiO2 supported mono- and bimetallic Au-Pd Nanoclusters for efficient photocatalytic H2 generation

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Abstract

Hydrogen production by photocatalytic process is a promising, clean, and environmentally friendly energy source to solve the energy crisis and environmental issue. Photocatalysts often composed of noble metal nanoparticles deposited on a semiconductor are capable of promoting hydrogen production from alcohols. Gold nanoclusters (Au NCs) with atomic precision have huge application potentials such as energy conversion. In this work, initially two different mesoporous black TiO2 (meso-TiO2) samples were synthesized using the sol-gel technique. Two different Pluronic triblock-copolymers (P123 and F127) were used as structure-directing agents in the sol-gel synthesis method. Later, mono- and bimetallic Au-Pd nanoclusters deposition on the surface of mesoporous black TiO2 samples was performed. The synthesized photocatalysts were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), nitrogen adsorption-desorption, Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), elemental analysis and (EA),), UV-vis diffuse spectroscopy (UV-vis DRS) techniques to investigate physico-chemical properties. The photocatalytic activity of the synthesized catalysts in hydrogen production will be correlated to structural, electronic and morphological characteristic properties of the catalysts.

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Nobel metal decorated graphitic nitride-mesoporous oxide heterojunction for photocatalytic hydrogen production

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Session: Catalysis -- Photo-Catalysis

ABSTRACT

In this research, it proposed to synthesize heterojunction of mesoporous CeZrO4 and graphitic nitride layered nanosheet structure and subsequent in-Suite photo-deposition of noble metal nanoparticles for successful utilization of the final material for photocatalytic hydrogen production. The Physico-chemical properties of the synthesized nanostructures will be studied using XRD, FTIR spectroscopy, Raman spectroscopy, TEM, DRUV-vis, XPS and N2-physisorption techniques. The results from powder XRD and spectroscopy results will be utilized to study the formation of different phases due the interaction between heterojunction. The aim of the research is to study the influence narrowing bandgap by exfoliation methods to increase the active site and functionalization to strong loading on the phase and morphology changes in the resultant nanomaterial. All the synthesized nanostructures will be utilized as catalysts for photocatalytic hydrogen production the Physico-chemical properties of synthesized nanostructures will be correlated with the reaction rates among the investigated samples.

Saudi Aramco: Company General Use

Micro-Algae Biofuel Production Facity at SA/Seawater Injection

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Session: Carbon Capture and its Applications

ABSTRACT

The Algae Biofuel Production Facility at QSWP, hosted by SWID, is Aramco's first such facility as part of the corporate Green Energy Program. The development of the facility will help plan for corporate expansion of this program by evaluating algae biofuel production levels throughout the year as affected by water parameters and weather.
SWID utilized an existing Sewage Treatment Facility (STP) ponds to construct the Algae farms that will be tested to produce Green energy low carbon biofuel. The initiative aims to demonstrate the sustainability potential of developing a new Green low energy intensity algae-based biofuel for Saudi Aramco to utilize in its planned new fuel distribution stations, and as part of its aviation, bus and car transportation fleet.
In addition, useful by-product of algae biofuel production such as Aquaculture and Livestock feed including providing valuable aquaculture fish food for the Saudi Aramco Fish Hatchery, and for the Kingdom’s expanding aquaculture Industry.
Algae is quick to grow and helps control environmental pollution by consuming carbon dioxide (CO2) emissions from atmosphere and may be pumped into the ponds. In just three to five days, algae also eliminates ammonia, a high percentage (above 85%) of nitrate, and about 99% of phosphate from wastewater which will support the QSWP Sewage Treatment Facility operation in eliminating ammonia and phosphate.
Algae biofuel produced by Aramco is projected to be the world's most sustainable biofuel which will reduce GHG emissions from the transportation fleet. The production process itself also acts as a carbon sink, as CO2 and NOx enhance algae productivity.
The environmental benefits will be reflected on both the Kingdom and the world. Aramco plans to make algae biofuel available for use at upcoming gas stations in the Kingdom and export for transportation use potentially at Europe.
The algae biofuel testing facility will become part of a permanent change of QSWP's seawater and wastewater treatment processes, potentially requiring up to 2.4 million barrels at anticipated upscaling capacity.

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Development of Cellulose Acetate-based Natural Fibers/Zinc Oxide Bionanocomposites as Efficient Adsorbents for Oil Spill Removal

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Session: Materials for Environment and Wastewater Purification

ABSTRACT

Development of Cellulose Acetate-based Natural Fibers/Zinc Oxide Bionanocomposites as Efficient Adsorbents for Oil Spill Removal

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ABSTRACT

With increasing usage of crude oil and its products, there has been a growing concern over oil pollution of environmental waters. As a result, there is a considerable need for the development of effective techniques and materials for cleanup and removal of oil from the environment. An oil absorbent made of lightweight porous material is one of the most promising solutions among others because it is extremely effective, environmentally friendly, and simple to use. The goal of this research is to create an efficient and environmentally friendly oil sorbent based the natural palm fiber incorporated with cellulose acetate biopolymer in different levels fiber loading (10, 20,30 % wt) and modified the surface composite with ZnO nanomaterials with various concentration (2,5,10 and 20 wt%) and it investigates the sorption capacity of raw and modified fibers for diesel oil. The fabricated materials have been characterized by common characterization tools. In this research, the effects of different palm fibers content and concentration of ZnO nanomaterials on oil sorption efficiency were quantified. Based on cellulose acetate

polymer, 30% wt natural palm fibers, and 10% wt ZnO nanomaterials the modified sorbents displayed about 2 fold increase in oil sorption capacity over raw fiber. The research revealed that the efficacy of fibers in removing oil from tap water was proportional to sorption time as well as system parameters such as oil volume, sorbent dosage, and pH.

Furthermore, the results showed that these sorbents had enough effectiveness, implying that they are suited for oil removal applications

Saudi Aramco: Company General Use

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Reduced Polymer Loading Fracturing Fluid for Extreme Temperature Applications

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Session: Industrial Chemistry -- Enhanced/Improved Oil Recovery

ABSTRACT

The main challenges associated with extreme temperature fracturing fluids for applications in the range of 350-400°F are the thermal-stability of the base polymer in this temperature range. Traditional hydraulic fracturing fluids that use crosslinked polysaccharide gels, such as guar and its derivative, are not suitable due to the significant polymer breakdown under these conditions. In this paper, a novel reduced polymer loading fracturing fluid, prepared using a novel thermally stable acrylamide-based terpolymer, is discussed for use in extreme temperature applications.

Thermally stable acrylamide-based terpolymer with reduced polymer loading of 30% less than guar-based fracturing fluid was considered to minimize formation damage concerns. A novel reduced polymer loading fracturing fluid was evaluated at 350°F with reduced polymer loading to 35 lb/1000 gal. For successful field implementation, reduced polymer loading fracturing fluid was evaluated in following sequence: chemical management and quality control, optimization of fracturing fluid formulations with field water, field mixing procedure, onsite QA/QC, friction analysis, leak-off analysis, data frac analysis, and execution of main fracturing treatment. The friction of crosslinked fluid was analyzed by using a bottomhole gauge, and fluid efficiency was evaluated during data frac analysis.

This paper presents rheological studies at bottomhole static temperature (BHST) and cool-down temperatures of selected well candidates that demonstrate superior thermal stability of this novel fracturing fluid. With polymer loading of 35 lb/1000 gal, the fluid viscosity stayed above 300 cP at 100 1/s shear rate for 1 hours at 350°F. The fracturing fluid formulations were optimized using both live and encapsulated breakers with a high pressure and high temperature (HPHT) rheometer. The main fracturing treatment was successfully executed with a 45-50 barrels per minute (bbl/min) pumping rate with increased proppant concentration up to 5 pounds per gallon (ppa) using 30/50 high strength proppant (HSP) proppant.

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Root Cause Analysis of Filter Sludge Deposits in Natural Gas Liquid Recovery Unit - A lab Case Study

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Session: Industrial Chemistry -- Petroleum Products

ABSTRACT

Abstract

This article reports a lab case study of the accumulated filter sludge deposits, frequently accumulate inside the equipment used in the oil industry, which can cause failures and temporarily shut down the gas plants, in natural gas liquid (NGL) Recovery Unit. Totally three different filter sludge samples were collected and conducted a lab case study by using Thermogravimetry analysis (TGA), X-ray powder diffraction (XRD), Gas Chromatography - Mass Spectrometry (GC-MS) and Environmental Scanning Electron Microscopy and Energy dispersive spectrometry (ESEM/EDS) analysis.

All sludge deposits were treated with dichloromethane (DCM) to separate the non-hydrocarbon part (or inorganic crystalline materials or non-soluble part) from the hydrocarbon parts (soluble part) of the accumulated filter sludge deposits.

The phase identification and quantification of whole-X-ray powder diffraction patterns of inorganic crystalline materials part of the corrosion products and/or desiccant materials are significantly important to accurately and precisely determine in order to prevent the reoccurrence of these particular solid deposits at the filters at various stages of NGL Recovery Unit.

Thermal gravimetric analysis (TGA) results revealed that the sludge sample-A (collected bottom of dehydration unit filters) contained approximately 14 wt% of inorganic compound

and 86 wt% of hydrocarbons. Subsequently, GC-MS analysis results revealed the presence of amines (methyldiethanolamine - MDEA and piperazine), elemental sulfur and C9–C25 hydrocarbons in Sample-A. In this paper, all three different filter sludge deposit samples were analyzed and discussed the possible reasons for accumulated deposits in NGL Recovery Unit.

The findings will help the investigation team to identify the possible root cause of the unknown materials and take corrective actions to avoid the reoccurrence of these deposits in the near future. The above prerequisite results which are required to facilitate chemical cleaning of the particular equipment in gas plants will be described in this paper.

Keywords: Filter Sludge deposits, Natural Gas Liquid (NGL), Gas Processing Plant, Elemental Sulfur, Organic Amines and Desiccants.

Saudi Aramco: Company General Use

Design and synthesis of organic semiconductor for photoacoustic imaging

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Session: Materials -- Functional Material Synthesis and Characterization

ABSTRACT

Photoacoustic imaging is a technique based on the photoacoustic effect, and it is proven to be reliable in achieving deep-tissue penetration without being exposed to ionising radiation.

This project's aim was the synthesis of a BBT conjugated small molecule that, upon subsequent coupling with a hydrophilic component, can be processed into water soluble nanoparticles for near-infrared photoacoustic imaging. The first part of the project consists of developing a semiconducting small molecule between an BBT □-electron acceptor and different □-electron donor and fusing it with a biocompatible component. The second part of the project consists of studying the twisting of the molecule to see whether it exhibits tict character.

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Widening the scope of polyolefin's composites applications with the use of low-cost fillers

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Session: NA

ABSTRACT

Low-cost mineral fillers represent interesting economically suitable alternatives for reducing composite cost and improving the mechanical performance. The use of CaCO3 and platy shape silicate mineral Talc as low-cost inorganic fillers along with selected additives showed promising results including tensile and flexural strength while maintaining cost reduction. The study results revealed different material formulations exhibiting the best balance between processability, volume cost and mechanical properties. The potential of CaCO3 fillers was evidenced for preparation of highly loaded up to 60 wt% reinforced composites, reducing volume-cost of materials by around 25%. The incorporation of Talc filler showed remarkable reinforcing effects, with particular interesting balance between flexural and tensile properties. Master batches were successfully used for preparation of demonstrator pallet prototypes at pilot scale with standard industrial injection molding equipment. Selected combinations would open new prospects in various applications in logistic, packaging, automotive and 3D printing domains.

Crosslinked Siloxane/POSS Organic-inorganic Nanocomposite Membranes for Enhanced C3+ Heavy Hydrocarbon Recovery from Natural Gas

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Session: Industrial Chemistry -- Polymer and Nano-Composites

ABSTRACT

Crosslinked Siloxane/POSS Organic-inorganic Nanocomposite Membranes for Enhanced C3+ Heavy Hydrocarbon Recovery from Natural Gas

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Natural gas is of strategic interest to Saudi Aramco, both to reduce the Kingdom's reliance on liquid fuel for power generation and to provide further economic growth and diversification. Heavy hydrocarbons (C3+), one of valuable chemical feedstocks, are conventionally separated through cryogenic distillation, pressure swing adsorption, or other energetically intensive refrigeration processes. Membrane-based separation technology has gained great industrial attention over the past years due to its environment-friendly and energy-efficient solution to the bulk separation of contaminants from natural gas. Commercially, PDMS based siloxane rubbery membranes have been applied to separate C3+ hydrocarbons from natural gas. However, conventional PDMS membranes exhibit low C3+/CH4 selectivities due to high degree swelling under hydrocarbon rich feed streams and operating conditions. Organic-inorganic hybrid membranes have been the subject of growing interest in recent years due to the combined properties of organic and inorganic system. In this talk, we describe a method to produce novel organic-inorganic nanocomposite membranes by incorporating a dual-functional nanofiller as a crosslinking agent and nanofiller within membrane matrix. A novel, dual-functional POSS nanoporous crosslinking agent consisting of silicon hydride moiety and trimethoxylsilicon groups attached to a central POSS core, was synthesized and characterized. Gas permeation properties were evaluated using pure gas and C3+

hydrocarbon rich multicomponent gas mixtures under varying operating conditions. Results show that crosslinked siloxane/POSS organic-inorganic nanocomposite membranes exhibited high swelling resistant and crosslinking density, and enhanced C3+ separation performance under simulated typical field gas testing conditions compared to conventional PDMS. At 800 psi, crosslinked siloxane/POSS hybrid membrane exhibited C3H8/CH4 and C4H10/CH4 selectivities of 7.7 and 18.7, respectively. This study provides useful insights in exploring and designing better rubbery siloxane membrane materials for actual industrial processes.

Saudi Aramco: Company General Use

Facile one-step green synthesis of gold nanoparticles (AuNP) using Licorice root extract:

antimicrobial and anticancer study against HepG2 cell line

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Session: NA

ABSTRACT

Nanostructures synthesis via green method has been popular due to agitating assets and ground-breaking applications. Cost-effective novel and environment friendly gold

nanoparticles (AuNP) synthesized via licorice root extract. The conditions for the eco-friendly AuNP synthesis was optimized by 6 mL salt concentration and 4 mL extract with pH 5 after 2:30

hours at 25℃ temperature. A more detailed characterization of green synthesized AuNP was performed using UV-Vis, Fourier-transform infrared (FTIR) and X Ray diffraction (XRD)

spectroscopy EDX analysis, transmission and scanning electron microscopy, DLS (dynamic light scattering) and High-performance liquid chromatography to identify the components within

licorice root extract. With the aim of retrieving consistent capacity on antioxidant activity ABTS and DPPH two dissimilar broadly applied antioxidant methods were applied. The cytotoxicity of

green synthesized AuNPs was assessed applying an MTT method upon MCF-7 (breast cancer), HePG-2 (liver) cell-lines. The antifungal with antibacterial activity of green synthesized AuNP was

examined by agar well diffusion technique. The as synthesized AuNP showed restrained antibacterial, antifungal activity towards bacterial and fungal strains used and importantly reflective

anticancer activity was observed against used cell lines.

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Nanostructures synthesis via green method has been popular due to agitating assets and ground-breaking applications. Cost-effective novel and environment friendly gold

nanoparticles (AuNP) synthesized via licorice root extract. The conditions for the eco-

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Abstract Ref Number: ID- 6413

Session: NA

ABSTRACT

Green synthesis and characterization of nanoparticles have became an important branch of nanotechnology In this study, an eco friendly green synthesis of the gold coated

iron Fe@AuNPs using extract solution of olive oil, licuorice root Glycyrrhiza glabra and coconut oil acted as a reducing agent during the synthesis of core shell nanoparticles at

ambient conditions i e long time stability, lower toxicity and higher permeability to specific target cells In order to achieve the small size 10 nm) with regularly spherical shaped and

homogeneous particles microwave irradiation were used which offers a higher reaction rate and better product The Fe@AuNPs have been characterized by UV Visible spectroscopy,

Energy dispersive X ray spectroscopy(EDX), X ray diffraction (High resolution Transmission electron microscope (HR TEM), Fourier Transform Infrared Spectroscopy (FT

IR) and high performance liquid chromatography HPLC), High angle annular dark field scanning TEM (HAADF STEM), Particle Size Distribution (Magnetic hysteresis loops

The synthesized gold coated iron NPs showed significant antioxidant potential with high rates of free radicl inhibition The NPs were also affected against Helicobacter pylori

H pylori peptic ulcer and wound healing Conclusion/Recommendations From this study, it is clear that (extract proved itself a potent reducing and capping agent during

the synthesis of Fe@AuNPs and also had a significant anti ulcer activity in animal models The extract is non toxic even at relatively high concentrations

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Biogenic Proficient Synthesis of (Au-NPs) via Aqueous Extract of Red Dragon Pulp and Seed Oil:

Characterization, Antioxidant, Cytotoxic properties, Anti-diabetic Anti-inflammatory, Anti-Alzheimer

and their Anti -proliferative Potential against cancer Cell

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ABSTRACT

Gold nanoparticles with tiny sizes and biostability are particularly essential and are employed in a variety of biomedical applications. Using a reducing agent and a stabilising agent to make gold nanoparticles has

been reported in a number of studies. Gold nanoparticles with a particle size of 25.31 nm were synthesized in this study utilising Hylocereus polyrhizus (Red Pitaya) extract, which functions as a reducing and stabilising agent. The

extract of Red Pitaya is said to be a powerful antioxidant and anti-cancer agent. Because of its substantial blood biocompatibility and physiological stability, green production of gold nanoparticles with H. polyrhizus fruit extract is

an alternative to chemical synthesis and useful for biological and medical applications. The formation and size distribution of gold nanoparticles were confirmed by HPLC, UV–Vis spectrophotometer, X-ray diffraction (XRD),

Dynamic light scattering (DLS), Zeta potential, Transmission electron microscopy (TEM), Fourier transformed infrared spectroscopy (FTIR), Energy dispersive X-ray (EDX) and X-ray photoelectron spectroscopy (XPS). The wellanalysed

NPs were used in various biological assays, including anti-diabetic, anti-inflammatory, anti-Alzheimer, and antioxidant (DPPH), and cytotoxic investigations. The NPs also showed a dose-dependent cytotoxic activity

against HCT-116, HepG2 and MCF-7 cell lines, with IC50 of 100 µg/mL for HCT-116 cells, 155 µg/mL for HepG2, and for MCF-7 cells the value was 165 µg/mL respectively. Finally, the outstanding biocompatibility of Au-NPs has

led to the conclusion that they are a promising choice for various biological applications.

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Ephedra mediated green synthesis of gold nanoparticles (AuNPs) and evaluation of its antioxidant, antipyretic, anti asthmatic, and antimicrobial properties

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ABSTRACT

The eco friendly green bio synthesis of Ephedra AuNPs was constructed from Ephedra plant extract The synthesis process was optimized using different volumes of Ephedra extract, 10 3 M

(HAuCl 4 3 H 2 O) solution, reaction temperature, time, and pH of the solution Where, 4 mL of Ephedra extract, 6 mL of 10 3 M (HAuCl 4 3 H 2 O) solution at 25 C for 3 h at a pH of 4 are showed the optimum

reaction parameters respectively The characterization of AuNPs was verified by UV Vis spectrophotometer, FTIR, microscopic techniques (HRTEM), Zeta potential, and X ray techniques (EDX,

XPS) The nanoparticles are extremely important materials in emerging the future sustainable technologies for the living beings The AuNPs were employed in biological assays where ABTS assay used to

investigate the antioxidant activity The in vivo study of AuNPs was executed to study the anti pyretic and anti asthma activities of Ephedra AuNPs Ephedra AuNPs of 1 3 nm to 15 6 nm size were achieved

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which have as importance as proficient to bind with the biological systems The Ephedra AuNPs prepared exploiting Ephedra extract which is considered to be influential anti asthma agent and antipyretic

agent reduced the fever by 83 3 at **32µg/g/day** Further the Ephedra AuNPs used to scrutinize the anti bacterial activities for Staphylococcus aureus Listeria moncytogenes Bacillus subtilis Escherichia

coli Pseudomonas aeruginosa and Salmonella typhimurium and anti fungal activities on Candida albicans, Aspergillus nigra and Aspergillus flavus The synthesized Ephedra AuNPs exhibited great potential

activities comparable to the standard drugs in case of Staphylococcus aureus Escherichia coli, Candida albicans with the zone of inhibition of 25 0 5 nm, 26 0 6 nm and 24 0 7 nm respectively It is believed

that the synthesized Ephedra AuNPs to be a hopeful option intended for diverse biological applications