Session 1

Abstract (#19280)

Title: Chemical Property prediction using Machine Learning

Authors: Kiran K. Yalamanchi, Francesco Tutino, M. Monge-Palacios, S. Mani Sarathy, Xin Gao

KAUST

Machine learning methods can be used to better estimate properties of chemical compounds or their mixtures. To this direction, some works were reported for few properties that are not investigated in detail. In this work, we concentrate in detail, a thermodynamic property for a class of hydrocarbon species. Accurate thermodynamic data of chemical species is essential for chemical kinetic models to predict the outcomes of complex chemical reactions. Quantum chemistry calculations and experiments can be used to determine all the thermodynamic properties needed; however, these are arduous and time consuming. In this work, we utilize machine-learning algorithms as a tool for quantitative structure property relationship (QSPR) analysis to predict standard enthalpy of formation for a class of reactants and intermediates (Alkanes, alkenes & alkynes) required to build kinetic models. Enthalpy data of alkanes, alkenes and alkynes is taken from literature after conducting an exhaustive survey. Artificial neural networks (ANN's) and Support Vector Regression (SVR) are chosen since they can capture very complex relationships between input and output vectors that are required to map complex properties over dissimilar classes of molecules. ANN and SVR are used with a two-level K-fold Cross Validation (K-fold CV) workflow. (1) one of which is used to determine errors over the entire dataset, and thus the performance of the method, and (2) the second is used to validate the search over a predefined hyperparameter grid. Various molecular descriptors consisting of the topological information of species are analyzed for the feature selection to input in to machine learning models. In the later part, various parameters of machine learning algorithms are optimized for accuracy using K-fold CV workflow. These models can be used to predict enthalpy of molecules with no accurate data in the literature. A comparison of estimated enthalpy of machine learning models with traditional group additivity model suggests that there is large scope of improvement that can be achieved by using machine learning models. Supplementing this, a perturb sensitivity analysis pointed out that enthalpy is correlated with descriptors that are not direct group counts. This work aims at predicting a thermodynamic property for neat stable compounds and thus lays foundation for the further works of predicting other thermodynamic properties and also that of radicals, transport properties leading to solve the challenge of predicting reaction rates.

Abstract (#19315)

Title: Machine Learning Approach for Prediction of Reaction Yield with Simulated Catalyst Parameters

Authors: Akira Yada.

AIST

Prediction of reaction yields by machine learning approach is demonstrated in tungsten-catalyzed epoxidation of alkenes. The various electronic and vibrational parameters of the phosphonic acids are collected by DFT simulation, and chosen by LASSO as the essential parameters for prediction of the reaction yields. With the trained model, we can predict yields of the reaction with unverified phosphonic acids with an error of 26%.

Abstract (#19342)

Title: A Machine Learning Approach for Pipeline Internal Corrosion: Retrospective and Prospective

Authors: Christian Canto Maya, Biswas Avidipto, Nasser Otaibi.

Saudi Aramco

Modeling pipeline internal corrosion has been challenging for pipeline operators. Recently, the combination of Artificial Intelligence algorithms has been viewed as an effective way to build reliable predictive models. To estimate the internal pit corrosion behavior of aged oil and gas pipelines and their subsequent maintenance an intelligent machine learning tool was utilized to develop an internal corrosion probabilistic model. The proposed model considers In-Line Inspection (ILI) data of multiple operating pipelines. The probabilistic model was incorporated utilizing machine learning tools. The proposed model is able to predict the maximum corrosion as well as the multivariable effect of operating conditions, pipeline characteristics, water chemistry, and elevation profile. To demonstrate the application of the multiple classifiers model, a case study of six lines exposed to wet sour crude conditions were selected and used for the development and validation of the proposed model.

Abstract (#19349)

Title: Cyber-Physical Approach for the Detection of Corrosion Under Insulation

Authors: Ayman Amer Ayman Amer, Ali Al Shehri, Vincent Cunningham and Ihsan Taie.

Saudi Aramco

Corrosion under insulation (CUI) is a critical challenge that affects the integrity of assets where the oil and gas industry is not immune. Its severity arises due to its hidden nature as it can often times go unnoticed.

CUI is stimulated, in principle, by moisture ingress through the insulation layers to the surface of the pipeline. In this work, we describe how common image processing techniques from infra-red images of assets can be enhanced using a machine learning approach allowing the detection of locations vulnerable to corrosion. The results and conclusions of this work on real field assets in operation demonstrate the feasibility of this technique to predict and detect thermal anomalies directly correlated to CUI. This innovative work has led to the development of a cyber physical that meets the demands of inspection units across the oil and gas industry, providing a real-time system and online assessment tool for CUI utilizing trending artificial intelligence technology.

Keywords: CUI, thermography, machine learning, Artificial Intelligence"

Session 2

Abstract (#19278)

Title: Small molecule activation using computational catalysis and data-driven approaches.

Authors: Yousung Jung

KAIST

Electochemical activation of small molecules (CO2, N2, etc) towards value-added products is an efficient and sustainable way to address energy problems and global climate changes. In this talk, I will discuss some of our recent efforts to understand and design new materials towards electrochemical catalysis using density functional calculations. In addition, solid state materials are often complex, but can also be potentially highly tunable if there is a way to accurately extrapolate the large set of existing data for a new discovery, an area in which machine learning can help significantly accelerate the discovery proces with improved accuracy. I will describe some of our recent efforts to use machine learning for chemical science that can contribute greatly to creating solutions to catalysis and materials problems for small molecule activation.

Abstract (#19295)

Title: Automated Kick Detection Using Data Mining

Authors: Raed Alouhali Salem AlGharbi, Abdullah AlYami

Saudi Aramco

Objectives/Scope:

Using advancement in data analytics and the huge amount of data generated while drilling to develop an automated system to detect kicks while drilling. Detecting kicks in early stages gives the crew ample time to control it resulting in a safer and more efficient drilling operation. Several models were developed and evaluated to optimize kick detection using surface parameters such as: pressure gauges, flow meters, hook load, rate of penetration, torque, pump rate, and weight on bit.

Methods, Procedure, Process:

We collected drilling data from drilled wells that had a well control incident during the operation. Then we reviewed and cleaned the data to build a training data set. Over one million instances were used to prepare the training data set. Each instance has fourteen attributes reflecting relevant drilling parameters. Ten-fold cross validation was used for testing each model. Overall, five models were evaluated they are: Decision tree, IBK nearest neighbor, sequential minimal optimization algorithm, Artificial Neural Network,

and Bayesian Network. The performance of these models were calculated and compared using metrics such as accuracy, precision, recall, m-measure, MCC, ROC Area, PRC Area, mean absolute error, root mean squared error, relative absolute error, root relative squared error and kappa statistic.

Results, Observations, Conclusions:

This research is incremental, with each addition to the training data set, the accuracy of the models increase. Decision tree had good results with an added benefit that it was easy to visualize and explain physically. However, the best performance of all 5 models is IBK nearest neighbor with a staggering 99.99% accuracy, and all other metrics such as recall, precision, m-measure, MCC, ROC, PRC greater than 90%. Out of one million instances, only 32 instances were incorrectly classified.

Novel/Additive Information:

Development of a new model and procedure to detect kicks real time while drilling with high accuracy. Detection rate and speed is high, giving the crew enough time to react to the kick and maintain the wellbore stability and mud rheology.

Abstract (#19322)

Title: SVR-CSA Based Platform for Modelling and Optimization of Waste Water Treatment by Chlorella Kessleri

Authors: S.M. Zakir Hossain, N. Sultana and S.A. Razzak

University of Bahrain

This study focuses on developing empirical models for predicting the removal efficiencies of two response parameters such as nitrogen and phosphorus from waste water by Chlorella Kessleri. These response parameters are mainly dependent upon temperature, light-dark (LD) cycle and nitrate-to-phosphate (NP) ratio. Two competing data mining techniques such as response surface methodology (RSM) with Box-Behnken Design (BBD) and support vector regression (SVR) are applied in developing the empirical models. The results demonstrate that the developed models are suitable for predicting the response parameters with a satisfactory goodness of fit. It has been found that SVR model is much better than RSM model for predicting the response parameters. Finally, crow search algorithm (CSA) (nature-motivated metaheuristic algorithm) coupled with SVR is utilized for global optimal solution. Best operating conditions are calculated to be: 20 oC of temperature, 14 h of LD cycle and 1.9:1 of NP ratio. The nitrogen and phosphorus removal efficiencies under these conditions are found to be 99.9 and 66 %, respectively.

Abstract (#19576)

Title: Data Management and Integration Framework for Industrial Internet-of-Things in Oil and Gas Smart Pl

Authors: Dr. Abdullah Al-Halafi

Saudi Aramco

In our modern age Industrial Revolution 4.0 (IR-4), Oil and Gas Smart Plants are foreseen to change the way production processes are performed. In this paradigm, data acquisition and analysis are treated more perceptively, rather than merely automation, control and monitoring by human interactions. Nevertheless, the introduction of Artificial Intelligence (AI) and Machine Learning (ML) would not be sufficient without the deployment of Industrial Internet-of-Things (IIoT). Those form key components in this Smart Plant Physical-Cyber connectivity, and data crowdsensing and management. However, developing an integrated system that can be merged seamlessly into existing network's infrastructures can be challenging. The IIoT is still in its infancy and deployments in large-scale plants with coexisting harsh and complex networks must be carefully considered. This work presents a comprehensive study on the deployment of IIoT in industrial plants, and the associated developments in communication technologies and standards. Further, the optimization and intelligence of processes, physical and virtual interactions, layout and design of wireless connectivity, remote diagnosis and programmability, safety, security, and environmental ecosystem are among many various aspects to analyze. The recommended framework will be discussed based on network middleware approaches, big data flow sensing, classification, and connection management, and energy efficiency of IIoT networks.

Session 3

Digital Transformation:

Abstract (#19291)

Title: Axens\'s Connect'In™ : Towards Connected Refineries with Advanced Unit Performance Management

Authors: Luc Wolff, Pierre-Yves Le-Goff, Ali Jahel.

Axens SA

The digital transformation in the refining and petrochemicals industries is becoming a top development priority in order to maximize value from existing assets, achieve higher operation flexibility and reduce operation costs.

Digital technologies allow new insights and information from existing data, which helps creating value to stakeholders and enhance the performance management of catalytic process units.

Axens has introduced very recently Connect'In™ to the market place: an interoperable "software as a service" or "SaaS" which has been developed with the objective to support process and operation engineers and managers in their decision making process and allow them to capture opportunities to get more value from existing units.

Connect'In is a natural evolution of Axens assistance services supporting our ambition to become the trusted advisor of our clients during the unit life cycle: At the heart of the Connect'In™ solution is the combination of expertise of Axens's technology specialists reviewing the data and high fidelity reaction models. It also embeds expertise coming from Axens's technical assistance experience on process units across the globe. This combination guarantees the quality of nformation and recommendations that are made available through Connect'In™ to support our customers in their decision process.

Connect'In™ solution is built on the three following pillars:

- Reliable data from operation that have been validated and reconciled in order to have a correct picture of the operation at any time of operation

- Access to Axens experts and high fidelity model for an accurate analysis of catalyst performances (activity, selectivity, life time). The high fidelity model based on Axens know-how and expertise allows normalizing data depending on unit operating conditions (severity, throughput, feedstock, etc;) during the entire cycle length and even between cycles, allowing highly relevant unit performances assessment.

- Web dashboard providing an overview of the Key Operating Indicators and Key Performance Indicators in accordance with customer operation and economic targets. The interface provides analysis for process, operation, planning engineers and managers.

What Connect'In™ does through the highest standards of cybersecurity:

- Automatically collect relevant process information, being interoperable with software solution or cloud already in place on your sites,
- Data conditioning and reconciliation,
- Analysis with advanced computation, prediction with high fidelity models and review by Axens experts,
- Taylor made dashboard according to site standards and best practices,
- Catalyst status follow-up after catalyst analysis in Axens Laboratory (specific to Reforming CCR)

This talk aims at introducing Connect'In™ and display several studies on Catalytic Reforming units where Connect'In™ simplifies operation, data management and analysis while maximizing profit in a wide range of situations.

Abstract (#19177)

Title: Bridge Safety & Security mandates for industrial process felicities (Energy Industry)

Authors: Khalid S. Alghamdi

Saudi Aramco

Industrial Control System (ICS) cybersecurity attacks is getting more complex every day. The latest TRITON, sometimes refer to as Trisis, malware attack imitated beyond other known industrial cyber-attacks. The technique of the attack was directly interacting with a Safety Instrumented System (SIS). SIS is designed as the last line of automated process safety defense for industrial facilities to prevent equipment failure and catastrophic incidents such as explosions or fire. As a result, the regulation and standard bodes start addressing this delicate balance between process safety and security. This paper provide an overview of IEC 61508, IEC 61511, and IEC 62443 standards that address safety and security design. The paper also provide the techniques to bridge the common design gaps between the two domains

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Abstract (#19347)

Title: Robotics in Oil&Gas Operations; A Review

Authors: Ahmed Alalouni, Muhammad Arsalan, Abubaker Saeed; Muqbil Khalaf.

Saudi Aramco

In the complex and demanding oil&gas environment, there is a continuous struggle to make the operations efficient and safe. oil&gas business face various challenges including safety, efficiency, and reachability to name a few. Robotics are expected to play a major role in addressing these challenges. This paper presents a comprehensive review of the applications of robotics in oil&gas operations.

In this paper the robots designed for oil&gas applications are classified based on their actuation mechanisms including electric, hydraulic, and pneumatic and are compared for their important characteristics including size, weight, payload, reachability, precision, and the degrees of freedom. Improving safety, efficiency, reachability, and timeliness are some of the important challenges in oil&gas that can be resolved by robotics. For example, drilling operations such as derrick, floor, and motor hand shifting work have integral safety challenges that increases the risk of injury to the operators. Drilling automation and rescue robots can reduce the safety constraints. Downhole sensing is one of the reachability challenges, where communication means from wellbore to the surface and the data transmission rates are the limiting factors. A logging robotic can eliminate these constraints. Seismic survey are one of the efficiency challenges, where thousands of geophones are deployed manually to record seismic data. Geo-sensor robots, and underwater robots can reduce this efficiency constraint.

A paradigm shift is happening with the application of robotics in oil&gas operations for automation, reach, and safety that will lead to the complete transformation of the operational landscape. This work establishes the state of the art with classification and comparison of the robotics in oil&gas.

A comprehensive review of the state-of-the-art in oil&gas robotics is presented in this paper. The robots are classified and compared with presented tables consists of different characteristics for reviewing robotics in oil&gas operations.

Abstract (#19517)

Title: Advanced Process Intelligence at Air Products Saudi Technology Center

Authors: Pratik Misra, Vijay N. Kumar, Umesh Patil.

Air Products

Air Products is a fortune 500 industrial gas company that operates in more than 50 countries running 750+ manufacturing plants and more than 1800 miles of industrial gas pipelines. Various digital technologies are being implemented in Air Products to move towards Industry 4.0 standards.

Air Products has opened a new technology center in the Kingdom in Dhahran Techno Valley in August 2018. As a part of this technology center, a process intelligence center has also been established. Various digital technologies within the industry 4.0 paradigm have been implemented in this center.

In this talk, an overview of the process intelligence center will be given. Examples of various technologies being implemented towards achieving digital transformation of Air Products operations in KSA will be shared.

Session 4

Abstract (#19382)

Title: Molecular Modelling of Co-processing Biomass Pyrolysis Oil with Vacuum Gasoil in an Oil Refinery Flu

Authors: Mohamed Al Jamri, Robin Smith; Jie Li.

University of Manchester

Integration of biomass resources in petroleum refining for sustainable production of transportation fuels has gained increased attention in the last few decades. One potential integration option is to mix biomass-based pyrolysis oil (BPO) with petroleum gas oil (VGO) and then co-process the blend in oil refinery fluidised catalytic cracking (FCC) units. For better understanding of the effect of reaction conditions, blending ratios and feed properties on product yield and quality, kinetic modelling of FCC units with co-processing of BPO and VGO is necessary. However, there are only limited efforts reported for such kinetic modelling. Although several approaches have been proposed for modelling of FCC units, they cannot be directly applied to modelling of co-processing BPO with VGO due to their inability to accurately characterise oxygenated molecules in the feedstock. True reaction routes and kinetics might be masked.

In this work, a novel molecular-level modelling approach is proposed for kinetic modelling of co-processing BPO with VGO in an oil refinery FCC unit. Molecular-level characterisation of BPO and VGO blends using Molecular Type and Homologous Series matrix is first conducted. Then, a novel reaction network is synthesized and a reaction model is developed for the proposed reaction network which considers not only the complex intermolecular interactions between various types of molecular attributes in the feed, but also the interactions between individual molecules and catalyst surface. A hybrid optimisation strategy combining genetic algorithm with SQP is developed to obtain the optimal parameters in the reaction model. The results demonstrate an overall good agreement between measured and predicted yields using the developed kinetic model for VGO: BPO blending ratio of 90:10, C/O ratio between 5 and 8, and reaction temperature of 525°C. PONA composition, oxygen compounds compositions and oxygen content in each product fraction such as gasoline, diesel and gas oil can also be predicted using the developed model. The effect of reaction temperature on product yields and compositions is investigated through sensitivity analysis and optimal product yield is obtained. The effect of different blending ratios of BPO and VGO on desired product yields, compositions, and qualities can also be investigated using the proposed model.

The proposed approach can be easily extended for modelling of other refinery units such as hydrocracking, offering potential opportunities to rigorously evaluate other integration options of biomass pyrolysis oil into oil refineries and obtain the optimal integration option of renewable resources such as biomass into transportation fuels system.

Abstract (#19453)

Title: Past, Present and Future Trends in Kinetic Modeling: Application to Hydrocracking

Authors: B. Celse, Per Julian Becker, Denis Guillaume

IFPEN

Transformation of heavy crude oil into more valuable light (naphtha) and middle distillates (kerosene and diesel) is becoming increasingly important for the refining industry. Hydrocracking plays a major role in this transformation. Development of models for industrial hydrocrackers has received a great amount of attention by the scientific community over the past decades. These models can be used for several targets: chose optimal operating condition in order to optimize one target (Real Time Optimization), carry out what if analysis in order to estimate the impact of feed variations… Depending on the target and the reactor to model (Hydrotreating or Hydrocracking), several models can be used from very simple (classical lumping) to much more complex ones (single events).

This paper proposes a global methodology including design of experiments and indicates the best models to use depending on the target (either first principles or machine learning models). Some examples from hydrotreating or hydrocracking will be provided (yields prediction, product properties prediction …)

It will also show the new trends regarding this topic by merging Machine Learning techniques with kinetic models techniques. It can be shown that the association of these two techniques can improve dramatically the obtained results either for yields or deactivation prediction.

Abstract (#19354)

Title: Computer-Aided Tool for the Uncertainty-Accounted Process Synthesis of CO2 Utilization Technologies

Authors: Jeehwan Lee, Jay H. Lee.

KAIST

CO2 utilization technologies continues to attract attention as a method of mitigating industrial greenhouse gas (GHG) emissions while simultaneously generating valorisable products. Despite these advantages, many CO2 utilization technologies are at a low technology readiness level (TRL), which is characterized by a lack of quantitative information and a large number of process design alternatives. A weak knowledge-base of these low-TRL technologies forces the reliance on first principle estimates and preliminary experimental data, both of which contribute considerable uncertainties that are difficult to quantify. This work aims to address this problem through the development of a computer-aided tool, TIPE-CUT (Tool for Integreated Process Evaluation of CO2 Utilization Technologies) for a systematic evaluation-based and uncertainty-accounted process synthesis. Evaluations for process synthesis involve

both technoeconomic analyses (TEA) of the process alternatives as well as a CO2 life cycle assessments (LCA) for global warming impact assessment. Both assessments are carried out simultaneously by utilizing a single inventory database provided by developed tool. The proposed framework involves a three step procedure whereby first, an inventory is established that includes all materials, utilities and services (transportation) involved in the process. In the second step, a superstructure network representing the process alternatives are generated. The modular step/interval model for superstructure networks allows for the integration of user-defined shortcut models into the mass and energy balances, while representing non-characterized processes as black-box units. The framework extends to include a Monte Carlo simulation algorithm for uncertainty propagation, which requires user-input with respect to the selection of Monte Carlo factors. The evolutionary algorithm minimizes the CVaR of the specific production cost (represented as $/functional-unit) and specific global warming impact (represented as ton CO2-eq/ton functional unit) with respect to the process alternatives as specified in the superstructure. CVaR minimization was selected over other metrics such as expected loss or VAR as it does not penalize positive deviations while averaging tail-end costs. The developed framework thus serves as a centralized evaluation platform, integrating aspects of both optimization-based process synthesis and stochastic uncertainty propagation. For policy makers, the tool can assist in the identification of R&D “hotspots” as well as setting and assessing target parameters for sustainable operation of CO2 utilization technologies.

Abstract (#19174)

Title: Development of a Novel Operating Plan for Khurais Steam and Fuel Gas

Authors: Abdulmohsin, Mohmmed T, Amminudin, Kamarul A

Saudi Aramco

The developed system and method are intended to solve the problems of the inherent limitation of the existing performance monitoring tool, which relies on the historical performance of the particular performance metric to make any related decision or action. The existing performance monitoring tool is more capable of identifying a problem ‘after the fact’. This reactive approach turns out to be costly and has a strong likelihood for an adverse impact on the operational safety. Preparing for the future operation, be it worse or better, by anticipating the likelihood of performance in the future operation is much more desirable. This is a proactive approach towards addressing comprehensive performance monitoring

Based on that concept, a new method and system were developed in-house to build an effective operating plan to ensure sustained optimum operation in the operating or process oriented facilities. The method is applied on the steam system at a Gas Oil Separation Plant (GOSP) to provide the operating plan. The tool adopts the advanced analytic modelling algorithm and optimization to provide the users (engineers and operators) with the recommended operating plan for the mode of operations in question for the next day, next week or next month. It involves two steps; namely the predictive and prescriptive phases. The first step allows the prediction of the performance be made based on the given historical performance

data, while the second step, utilizing the predicted performance data, employs the optimization algorithm to prescribe the predicted optimum performance. With this tool, by being proactive, the tool has guided the users to sustain optimum performance and specifically, during the deployment of the tool in the steam system, the fuel gas savings of around 1 MMSCFD ($ 2MM/year) were captured. Furthermore, by leveraging on this tool, the users are better equipped with a sound strategy for their next day of operation as they are now able to at least anticipate what to expect in the immediate future operation and to ensure their readiness of any eventualities during the operation to make the operation safer and reliable all the times.

Session 5

Abstract (#19273)

Title: A Rapid Technique to Quantify Stabilizer in Polypropylene

Authors: Lohith M N, Dr.Saeed Al-Shahrani , Dr.George Kuriakose, Sang Kim, Michael Hall, Faisal Al-Suhaibani, Abderrahman Meddad

SABIC

Irganox®1330 (1,3,5-Trimethyl-2,4,6-tris(3,5-di-tert-butyl-4-hydroxybenzyl) benzene) is a sterically hindered phenolic antioxidant that protects organic substrates against thermo-oxidative degradation. The content of this additive in the polymer is significant in determining the end properties like dielectric strength, compatibility to substrates and resistance to extraction. Thus, quantification of the additive is critical to quality. The additives are traditionally characterized by separation techniques, and HPLC is generally the first choice for the trace analysis of heat stabilizers like Irganox®1330. However, these methods are highly time consuming. Hence, alternatively developed a rapid quantitative FTIR method to quantify the levels of Irganox®1330 in polypropylene (PP).

The FTIR method utilizes the Infrared absorbance of characteristic hydroxyl group band associated with the Irganox® 1330. The developed calibration shows correlation coefficient (R2) >0.99 with low standard error of prediction which can be utilized to determine the additive content range of 500ppm to 3000ppm.

Abstract (#19558)

Title: Catalyst Characterization for Converting Heavy Compounds C9+ to BTX

Authors: Ibrahim Zaharni, Noor Mana and Ibrahim Jadidi.

Saudi Aramco

Heavy compounds (HC), containing C9+ aromatics, is the fraction that remains after extraction of the more valuable BTX (benzene, toluene, xylene) fraction from the catalytic reformate or the pyrolysis gasoline. This fraction was directly added to the gasoline pool. However, due to the restriction of the benzene content in gasoline by environmental regulations, it is important to find alternative ways of upgrading this stream into other valuable products. One option is to convert the heavy aromatics into additional BTX compounds. Simultaneous dealkylation and transalkylation reactions are utilized for converting low value products (heavy compounds) to high value products such as BTX. Several commercial catalysts have been modified and tested for converting low value products (heavy compounds) to high value products (BTX). Advanced analytical instruments such as (XPS, TEM, ICP, XRD and FTIR) have been used to characterize the developed catalysts and the data obtained by these instruments have been used to select the suitable

materials for catalyst synthesis, optimum conditions for catalyst testing and confirm the modification methods as well as understand the reaction mechanisms.

In this presentation, I will share the following points:

- Introduction of the project including objectives and achievements
- Methods for producing catalysts and their applications for heavy compounds C9+ conversion to BTX
- Reaction mechanisms for converting heavy compounds C9+ to BTX
- Different between commercial catalysts, modified catalysts and new catalysts for converting heavy reformate to BTX
- The advantages of catalysts, feeds and products characterization using advanced instruments such as (NMR, XPS, ICP, TEM, GCs and FTIR) for :

? material selections

? catalyst selection

? conditions optimizations

? understanding the reactions mechanism

- The results obtained by advanced analytical instruments

Abstract (#19383)

Title: X-Ray Fluorescence (XRF) for Monitoring and Controlling The Fabrication and Use of Catalytic Materia

Authors: Nagmeddin Elwaer, Nouri Hassan, Dev Ranjan Perdhan.

SABIC

The science and technology of catalysis is of great significance as it affects our daily life. Four major sectors of the world economy; petroleum and energy production, chemicals and polymer production, food industry and pollution control, involve catalytic processes. Catalysts are used to produce fuels such as gasoline, diesel, heating oil, fuel oil, etc. Production of plastics, synthetic rubbers, fabrics cosmetics, involves catalytic processes. Catalysts are also used in the production of the polymers including adhesives, coatings, foams, textile and industrial fibers.

Catalyst dosing and activity tuning are essential for achieving the best product quality using minimum reaction time and process energy. X-Ray Fluorescence (XRF) Spectrometer is an essential tool for monitoring and controlling the fabrication and use of catalytic materials in petrochemical plants. In this study, the role of XRF in characterizing different types of the catalyst including sensitive-to-air catalyst material is illustrated. The advantages and disadvantage of glass beads fusion and pressed pellets XRF

sample preparation methodologies are compared for characterizing the catalyst material. Accuracy and precision of the catalyst analysis using the XRF technique are compared to other analytical techniques such as AAS and ICP-OES.

Abstract (#19455)

Title: Achieving the highest accuracy of Helium measurement

Authors: Ahmed J. Ibrahim, Leroy Ellis, Steve Clayton, Hussain A. Shammary.

Saudi Aramco

Global Helium usage has witnessed constant and increasing demand due to its versatile utility for many technology applications. Helium is found associated with petroleum natural gases and recovered in refineries using specialized techniques where inherent concentrations prove economic to do so. Consequently, to prove an economic resource and determine the appropriate recovery technology application, it is critical to achieve the highest accuracy possible when measuring Helium concentrations in natural gas. To achieve this requires specific and advanced instrumental equipment, standards and analytical protocols to be implemented and maintained.

During setting up of a dedicated Helium laboratory, it was discovered that data from different laboratories and different Helium standards employed could reveal as much as a 20% error in measurement. This appears to be a result of the fact that Helium concentrations in natural gas are typically two to three orders of magnitude lower in abundance relative to hydrocarbon gas components such as methane or non-hydrocarbon components such as carbon dioxide and nitrogen and resulting errors in standard concentrations are magnified. Other observations also revealed problems may be related to slow leaks in gas sample bottles attributed to faulty valves and reactivity of some gas components during storage that resulted in undesirable gas artifact generation. Important problems such as these were observed, recognized, solutions developed, applied and ultimately solved with significant lessons learned."

Session 6

Abstract (#19404)

Title: Characterization of Synthesized Nano-Sized ZSM-5 Zeolite Catalysts by Using X-ray Powder Diffraction

Authors: Rasha A. Al-Ghamdi Husin Sitepu, Lianhui Ding, and Hassan M. Sadiq.

Saudi Aramco

In this paper, various nano-sized ZSM-5 zeolite catalysts with high crystallinity and yield were successfully synthesized in-house by various techniques. Subsequently, the high resolution X-ray powder diffraction (XRD) data were measured, and the purity and crystallinity percentage were determined by High Score Plus software. Furthermore, 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 [1, 2] has been extended to describe crystal structure of nano-sized ZSM-5 zeolite catalysts.

The results revealed that these zeolite catalysts mainly consist of ZSM-5, which has an orthorhombic crystal system with the space group of Pnma. Additionally, the crystallinity percentage ranges from 41% to 95% relative to the commercial ZSM-5 zeolite catalysts. Moreover, the silica/alumina molar ratio ranges from 24 to 85. Furthermore, the structural refinement parameters obtained from the Rietveld refinement with the generalized spherical harmonic description agreed well with the corresponding single crystal structure. The findings help to (i) obtain the targeted zeolite catalysts prior to the catalytic test, and (ii) develop the performance of the synthesized catalysts such as higher BTX yield, sulfur resistance, and feed flexibility compared to those of the commercialized benchmark catalyst, which will be benefited economically.

Abstract (#19263)

Title: Quantitative Rietveld Phase Analysis of Sludge Deposits from Refineries and Gas Plants

Authors: Husin Sitepu, Rasha A. Al-Ghamdi

Saudi Aramco

Sludge deposits — that accumulate inside oil industry equipment — can cause failures and temporarily shut down refineries and gas plants. Recently, Sitepu and Al-Ghamdi (2019); and Al-Ghamdi and Sitepu (2018) described a new method to separate the non-hydrocarbon part (i.e., crystalline inorganic materials) from the hydrocarbon part (i.e., dichloromethane soluble) of the sludge deposits. Also, the

researchers quickly and accurately identified the phase identification of X-ray powder diffraction (XRD) data of small amounts of crystalline inorganic materials, and performed quantitative Rietveld Phase Analysis for each of the identified phases. The method is fast and can accurately identify very small quantities of inorganic materials present in the sludge deposits.

In this paper, the method developed by Sitepu and Al-Ghamdi (2019) was extended to perform Quantitative Rietveld Phase Analysis of crystalline inorganic materials from: (i) a regeneration overhead acid gas condenser, (ii) water drawn off a pump's suction strainer in a gas plant, and (iii) inside the vessel's equipment of the sulfur recovery unit (SRU). The results revealed that the major phases are: (i) iron sulfide corrosion product with the hydrocarbon type of mixture of diesel and lube oil for sludge deposits from a condenser, (ii) calcium carbonate with the hydrocarbon type of lubricant oil for sludge deposits from a suction strainer for pumps, and barium sulfate with no organic hydrocarbon or polymer for sludge samples from a water recycling pump.

Moreover, the major phases for the small amount of crystalline inorganic materials, from different locations inside the vessel's equipment of the SRU, revealed that iron oxide corrosion products are found in the steam drum, and iron sulfate corrosion products are built up in the condenser. The presence of dissolved oxygen in the boiler feedwater is indicated by a high weight percentage of iron oxide corrosion products in the form of magnetite (Fe3O4), which appeared in the deposits collected from the steam drum. It is essential to quickly and accurately know the phases and their weight percentages of the small crystalline inorganic materials (non-soluble part) of the sludge deposits, along with the type of hydrocarbon soluble part. This knowledge can guide the field engineers at the refinery and gas plants, to facilitate efficient cleaning of the equipment by drawing up the right pro¬cedures, and take preventive action to stop the generation of those particular sludge deposits.

Abstract (#19374)

Title: Understanding the Factors in test method affecting the Measurement of Flexural Modulus of Plastics

Authors: Visvanathan Balasaravanan, Dr. Saeed Al-Shahrani.

SABIC

The flexural modulus or the modulus of elasticity in flexure, is one of the vital datasheet properties to understand the materials stiffness and resistance to bending force. The measurement of flexural modulus, governed by ISO 178, is critical to quality of the plastics and the measurement, in turn, is affected by testing conditions and sample molding. In this study, the various testing parameters which affect the flexural modulus are analyzed in detail to bring in better understanding to each of its contribution to the variation in the flexural modulus. The factors such as preload and speed of preload application, changes in load cell capacity, testing speed change, span length reduction, formulae used for calculating the modulus and dimensional changes of the specimen, are varied with a 3-levels change and the corresponding changes in flexural modulus values are recorded. Using six sigma methodology and statistical tools, the above factors were identified and further analyzed for how each affects the flexural modulus. The changes to the modulus were categorized into statistical differences through tools such as

one-way ANOVA and also checked whether the data falls within the predetermined upper and lower control limits. This study focused on the above factors which are either not defined for the test method or varied the factors to levels allowable within the standard to conclude whether it contributes to statistical significance to the flexural modulus. Parameters such as the preload and the preload speed caused statistically significant changes to modulus. On the contrary, the changes in test speed within the allowable tolerance of the governing standard did not show any difference in the modulus values and were within the control limits.

Abstract (#19304)

Title: Headspace Sampling Procedure for Difficult Aqueous Matrices Followed by GC-MS with Simultaneous FID

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In processing chemicals at various plants withing Sabic, quite some water streams are used. The analysis of the impurity content in process water is, undoubtedly, one of the most challenging analytical tasks that a laboratory can get involved in. Usually, the level of contamination needs to be checked prior to discharge or re-use. In that respect, especially the compounds with low volatility play an adverse role. What makes analysis of the aqueous streams - such as cooling water, condensed steam and scrubber water - complicated? There are various factors to be considered. There is a huge number of potential analytes varying in volatility, structure and polarity. One has to consider the concentration levels for which answers have to be provided in the ppb – high ppm range.

Although modern analytical GC instruments provide sensitivity, selectivity and speed, enabling a large analytical scope in terms of both analytes and matrices, still aqueous samples cannot be injected directly. Either the water itself is not compatible with the injection device and the column chemistry, or, high-boiling compounds present in the sample will foul the injection device. Various time-consuming and laborious sample preparation solutions have been provided over the years that resolve the above problems. In this lecture we present a strategy to analyze difficult water streams. An amount of up to 15 ml is heated in a commercial Head Space Sampling (HSS) system up to 140°C. The volatiles in the sample go into the head space, leaving high-boiling components and large molecules behind. In this way, compounds having a partial pressure at 140°C will go into in the gas phase.

The lecture will present data from a study in which temperature, volume, equilibration time and sample type were varied. Quantitative aspects were studied with respect to recovery, linearity, and limits of detection. A commercially-available mixture of 54 analytes was used to represent the various classes of compounds that can be found in the samples commonly provided to our laboratories. The use of a unique instrument that combines HSS with GC-MS with simultaneous FID was very beneficial is obtaining identification and quantitative data at the same time.
