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ABSTRACT BOOK

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ORAL PRESENTERS

POSTER PRESENTERS

1) FLAMMABILITY STUDIES BY CONE CALORIMETER ANALYSIS OF SILICA CROSS-LINKED POLY(METHYL METHACRYLATE)

PRESENTER: Lubna Ahmed[1], Ruiqing Shen[3], Logan Hatanaka[1], Bin Zhang[1], Sam Mannan[1,*], Zhengdong Cheng[2], and Qingsheng Wang[3]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

The widespread application of polymers in the domestic and industrial life of people necessitates the study of its flammability properties. Polymer, being hydrocarbon, is a potential source of fuel in any fire scenario. Flame retardant nanofiller can be one potential barrier to deteriorate the flame spread on the event of a fire. In the present study, silica nanofiller have been embedded via in-situ method within the poly (methyl methacrylate) (PMMA) matrix for forming fire retardant polymer nanocomposite. Polymer-nanocomposite have been chosen since they have demonstrated improvement in terms of thermal and mechanical stability, optical and electric properties when compared to the micro and macro varieties. To study the flammability properties and analyze the reaction of the same to the fire, cone calorimeter has been used. Fire reaction properties, such as Heat Release Rate (HRR), time to ignition, ignitibility, carbon dioxide yield, carbon monoxide yield, fire growth rate, total heat evolved (THE), Specific Extinction Area (SEA) etc. have been measured and compared for the neat polymer and polymer nanocomposite. There has been a reduction of 17%, 35% and 39% in peak heat release rate for 1 wt%, 2 wt% and 4 wt% silica crosslinked PMMA respectively compared to neat PMMA. There has also been reduction of THE and mass loss with the application of flame retardant materials owing to char formation.

2) CONDUCTING BLOCK COPOLYMER BATTERY ELECTRODE BINDERS COMPARED AGAINST THEIR HOMOPOLYMER BLEND ANALOGS

PRESENTER: Hyosung An[1], Xiaoyi Li[2], Cody Chalker[3], Maria Stracke[1], Rafael Verduzco[2,4], and Jodie L. Lutkenhaus[1,5]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

Electron- and ion-conducting block copolymers have been explored as battery electrode binders as a means to enhance both electrochemical and mechanical performance. The question remains as to whether the block copolymer architecture is truly necessary or how the block copolymer compares against an analogous homopolymer blend. Here, we explore this question by blending a diblock copolymer bearing electron- and ion-conducting blocks, poly(3-hexylthiophene)-block-poly(ethyleneoxide) (P3HT-b-PEO), with V_2O_5 to form an electro-mechanically stable hybrid electrode. These are compared against similar electrodes that contain P3HT and PEO homopolymers of similar molar mass. It is found that the homopolymer blends suffer from poor electrode morphology, leading to subpar performance. In contrast the diblock copolymer binder is superior as phase separation is discouraged and the electrode exhibits a more homogeneous structure. The electrode with P3HT-b-PEO has the highest capacity of 190 mAh/g, whereas V_2O_5 is only 77 mAh/g at a C rate of 0.1 after over 200 cycles. P3HT, PEO, and the blend have capacities of 139, 130, and 70 mAh/g, which are not nearly as impressive as the block copolymer binder.

3) A NOVEL METHOD FOR DERIVATIVE-FREE OPTIMIZATION BASED ON PARAMETRIC APPROACH

PRESENTER: Ishan Bajaj and M. M. Faruque Hasan

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, 77840

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Many practical engineering problems are multi-dimensional, computationally expensive, and may not have explicit functional forms/expressions of the objective function/constraints. Examples include optimization of process operations described by high-fidelity models such as computational fluid dynamics, partial differential equations and flowsheet simulation. The algebraic form of the objective function in these problems is unavailable and these can be referred as black-box problems. Although detailed process models have been useful for combining atomistic scale to process scale, the computational costs of using gradient based solvers are high. As a result, there has been a growing interest in derivative-free optimization (DFO), both in theoretical advancements and applications. It is assumed in DFO that evaluation of a black-box function is possible but expensive. One goal in solving these problems is to find the optimum of the original problem using as few function evaluations as possible.

An optimization method is proposed to solve a multi-dimensional black-box problem based on the projection onto a special 1-dimensional space. A univariate function on this space exists such that its optima corresponds to the optima of the original multi-dimensional problem. Based on sensitivity analysis, we provide useful properties of the function and geometric intuition on the conservation of the optima. A transformation matrix can be recursively applied to obtain this 1-dimensional function and transform back to the original n-dimensional space. A two-step iterative algorithm is also proposed to find the optima. The preliminary theoretical development shows promise to use this approach to effectively solve multi-dimensional black-box problems. The method is applied on a test suite of box-constrained problems and compared with 5 existing solvers. The results show that the proposed method performs superior compared to 4 of the solvers when the number of evaluations are limited.

4) CO_2 CAPTURE AND CONVERSION TO CHEMICALS VIA SYNGAS: SUPERSTRUCTURE-BASED PROCESS SYNTHESIS, MODELING, AND OPTIMIZATION

PRESENTER: Priyadarshini Balasubramanian[1,2], Ishan Bajaj[1,2], M. M. Faruque Hasan[1,2,*]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

Carbon dioxide is one of the key greenhouse gases emitted by human activities at the global scale and its primary source is the burning of fossil fuels for energy. Global CO_2 emissions in 2013 increased by 2.2% over 2012 levels to 32.2 Gt CO_2 and electricity and heat generation sectors contributed to nearly two-thirds of the emissions. Significant efforts have been made in the past to develop CO_2 capture and sequestration (CCS) technologies. However, large-scale CCS is still not deployed for reasons including high cost, technological barriers and uncertainty in geological storage. A promising alternative to CCS is to convert CO_2 to value-added chemicals via syngas (CO and H_2), which is an intermediate for many hydrocarbon-based fuels and chemicals. As much as 2 Gt/yr of fuels and 200 Mt/yr of chemicals can be produced from CO_2 utilization. In this work, we explore alternative technologies and routes for the thermochemical conversion of CO2 to syngas. We postulate a flowsheet superstructure with various alternatives for separation, conversion and upgrading. We allow both pure and dilute raw materials, such as CO_2 from flue gas, methane from stranded sources, oxygen from air and water, and hydrogen from renewables and other sources. A novel feature of our superstructure is that it includes integrated systems that perform separation and reaction in one unit. One such example is the inclusion of a tri-reforming membrane reactor which, instead of using pure CO_2, uses the mixed flue gas as feed, produces syngas, and separates nitrogen from the product at the same time and does not require separate CO_2 capture section at the upstream. For each alternative, we develop a rigorous model detailing the transport and kinetics to accurately predict the process performance. We use nonlinear algebraic and differential equation

(NADE)-based plug-flow reactor (PFR) models to describe various alternatives for CO_2 reforming (e.g., steam methane reforming, dry-reforming, tri-reforming, partial oxidation, and variants of combined reforming). These 1-D heterogeneous models are highly accurate in predicting the performance of the reactor. Through detailed simulation and comparison of stoichiometric, equilibrium and PFR models, we show that it is important to consider rigorous models to accurately predict the CO_2 conversion. Using the rigorous simulation platform, we also develop efficient surrogate models for the reactor outlet conditions as it changes with reactor type, design and operating conditions. The replacement of the NADE models with their algebraic surrogates allows us to pose the overall synthesis problem as a mixed-integer nonlinear optimization (MINLP) problem, which we solve to optimality. Apart from the overall process synthesis model, we also optimize the individual reactors to study the maximum conversion of CO_2 for that reactor at different desired syngas ratios. For the superstructure optimization, we consider different objectives such as maximizing the overall utilization of CO_2, minimizing the total annualized cost, and maximizing profit. We also take into account the auxiliary carbon dioxide emissions associated with various processing tasks in the network. In this presentation, we will discuss our overall synthesis framework and the optimization results.

5) PROCESS MONITORING OF NONLINEAR INDUSTRIAL PROCESSES USING MULTISCALE REPRESENTATION OF IMPROVED KERNEL PARTIAL LEAST SQUARE (KPLS) TECHNIQUE

PRESENTER: Chiranjivi Botre[1], Majdi Mansouri[2], Mohamed N. Nounou[3], Hazem N. Nounou[2] and M. Nazmul Karim[1]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

Process monitoring is an important aspect in the chemical industries to ensure safe and proper operation and to maintain process efficiency at the desired level. Data based process monitoring technique have been successfully applied where accurate process model is not available. In this work we have proposed Multiscale Kernel Partial Least Square (MS-KPLS) based moving window generalized likelihood ratio test (MW-GLRT) for the fault detection and diagnosis.

Partial Least Square (PLS) is a popular input output type fault detection model but this technique can be effectively applied mostly to linear processes. Kernel extension of PLS provides an effective technique for fault detection of nonlinear industrial processes. Being an input output model, KPLS can also used as nonlinear regression technique. Selection of kernel function and its parameter have a significant impact on the fault detection performance of the KPLS algorithm, therefore in this work we have proposed optimized kernel PLS to enhance the fault detection performance by performing multi-objective genetic algorithm optimization to minimize missed detection rate and false alarm rate. Wavelet function based multi-scale representation further enhances the kernel method due to its ability to effectively separate the deterministic and stochastic features of the data and has the ability to handle the noise, non-normal distribution and auto-correlated data set. Fault detection decision is based on the statistical test that is performed on the residue obtained from the developed model. Composite hypothesis method like generalized likelihood ration test (GLRT) shows superior fault detection performance over convention methods like T^2 test and Q^2 test, in this work we have used moving window based GLRT technique for fault detection.

The proposed MS-KPLS based MW-GLRT methodology fault detection performance is illustrated through Tennessee Eastman process problem (TEP), which is a continuous process problem based on Eastman chemical company. The fault detection results demonstrate effectiveness of the developed methodology with lower missed detection rate and false alarm rate.

6) TORQUE-DEPENDENT MOTOR REMODELING AND MECHANOSENSING IN E. COLI

PRESENTER: Ravi Chawla, Katie M. Ford and Pushkar P. Lele

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Bi-directional flagellar motors rotate helical filaments in Escherichia coli to propel the cell. Each motor comprises of a torque-generating stator complex and a rotor that consists of a molecular directional-switch. We showed previously that the stator-complex is responsible for surface-sensing, an ability that is likely involved in triggering swarming-motility. The stators remodel in response to perturbations in the viscous loads, and we hypothesized that the underlying mechanism is torque-dependent. That is, the amount of torque generated by individual units regulates the affinity between the stator-unit and the rotor. FliL, an inner membrane protein, has been reported to be important in the stabilization of torque-generation, at high viscous loads. As a result, fliL mutants are generally defective in swarming motility in several bacterial species. We employed dynamic and steady-state cell-tethering experiments to test whether torque regulates stator-binding in strains lacking FliL. Our results suggest that the loss of FliL has no effect on stator-remodeling at near stall loads. At low loads, direct tests of fliL mutants and wildtype cells confirmed previous results that suggested only minor differences in the swimming speeds. We will discuss how these results can be interpreted to test the torque-dependency hypothesis for remodeling and motor-mechanosensing.

7) CUMULATIVE RISK ASSESSMENT MODEL TO DETERMINE INCREASED RISK DUE TO IMPAIRED BARRIERS

PRESENTER: S. Zohra Halim and M. Sam Mannan

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Several barriers may work conjointly to reduce risks to acceptable levels and prevent major accident hazards. Such barriers may be technical, operational, human or organizational. However, it may not always be possible to immediately identify and repair/replace impaired or dysfunctional barriers due to various deviations including delayed maintenance, aging assets, improper procedure, management changes and insufficient competency. Evaluating multiple deviations and their associated cumulative risk remains a challenge given that systems are complex with non-linear interaction, dynamic, possesses component dependency and there is uncertainty in parameter estimation. Current research focuses on the roadmap to development of a model that will enable integration of the various kinds of deviations in a complex system for cumulative risk assessment to help make decisions to reduce risks to ALARP.

8) DESIGN AND OPTIMIZATION OF MODULAR TECHNOLOGY FOR INTEGRATED CARBON CAPTURE & CONVERSION OF CO2 USING METHANE SOURCES

PRESENTER: Shachit S. Iyer, Ishan Bajaj, Priyadarshini Balasubramanian and M. M. Faruque Hasan

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

A modular process is proposed for direct utilization of CO_2 from dilute sources using low-cost and unconventional methane to produce high-quality syngas – a precursor for many value-added chemicals and liquid fuels. Existing CO_2 utilization involves an isolated and a priori CO_2 separation which incurs high energy penalty and cost to power plants. A multifunctional and integrated process is developed that is capable of simultaneous capture and conversion of CO_2 from flue gas using natural gas or fuel gas from the same plant, or using nearby unconventional and distributed sources such as biogas or landfill gas. The technology is shown to be robust, can handle different feedstock compositions, and is suitable for distributed manufacturing of syngas. In this work, a conceptual design is presented and further intensified using first principles-based high-fidelity process model. Trade-offs and interactions between the

capture and conversion compartments are elucidated via detailed process simulation at certain conditions. A constrained black-box optimization method is employed to achieve more than 92.03 % CO_2 utilization at an operating cost of $97.74 per ton of syngas.

9) RESILIENCE-BASED LOSS OF CONTAINMENT (LOC) EVENTS PREDICTION ANALYSIS FOR POLY VINYL CHLORIDE PROCESS SYSTEM: UNCERTAINTY QUANTIFICATION

PRESENTER: Prerna Jain and M. Sam Mannan

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

In the oil and gas industry with changing technology and increasing regulatory standards, process safety and risk management has become challenging. There are uncertainties in the process systems operations. Questions such as, what is the right frequency of a process upset or an incident, what are the uncertainties involved in the process unit, can we predict incidents, how vulnerable is the facility for unforeseen stresses or conditions, are yet to be explored and answered. Also, systems are complex and deteriorate gradually with time or due to exposure to unexpected disturbances or events. It is important to understand the complexities involved and develop methods considering both technical and social aspects to make the system survive, adapt and organize into new configurations as per demand.

This need calls for the development of a holistic and integrated systems framework for effective risk management. The application of the resilience engineering perspective is gradually being explored as an approach for considering the dynamics of socio-technical aspects based on systems theory. The resilience methodology emphasizes on dynamics, consideration of existing and new types of threats, uncertainty, systems degradation and complex interactions. A combined framework for predictability, survivability and recoverability dynamic analysis is introduced with resilience metrics. This work establishes and presents typical scenarios of Loss of Containment (LoC) events and resilience metrics for batch plant operations. This paper presents a resilience-based approach to quantify uncertainty in the Poly Vinyl Chloride (PVC) process system to predict loss of containment events. Three types of uncertainties have been considered in the example – cooling medium temperature, agitator failure and reactor charging. For typical risk analysis data, the uncertainty probability distribution has a large variance. With this prior specification we use Gibb's sampling (a MCMC – Markov chain Monte Carlo technique) for posterior inference on the parameters. The results illustrate that with the use of resilience metrics data, the variance in probability distribution of uncertainties involved decreases. This work elucidates the complex interactions between social and technical components of process systems and their impact on the loss of containment events occurrence.

10) MODIFIED MICROFLUIDIC FLOW SYSTEM FOR ASSESSMENT OF MICROBIOLOGICALLY INFLUENCED CORROSION

PRESENTER: Susmitha Purnima Kotu, Sam Mannan and Arul Jayaraman

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Microbiologically influenced corrosion (MIC) is a multi-billion dollar problem impacting several industries. MIC often develops as a result of biofilm formation by multiple microbial species. There is no single mechanism to explain how MIC manifests itself at various impacted sites. Hence, development of effective mitigation strategies for MIC requires a thorough laboratory understanding of the corroding system. Several of the flow systems used for laboratory evaluation are either batch systems or require large amounts of corrosive waters. The modified microfluidic flow system to investigate MIC overcomes these disadvantages. In addition, this flow system is a once flow through system very similar to the conditions in a pipeline. This flow system on a small chip can be used to monitor biofilms and corrosion using confocal microscopy and electrochemical impedance spectroscopy. In addition, surface profile

measurements with scanning electron microscopy are also attainable with these small chips. These microfluidic flow systems can be used for two applications-consortia studies and evaluations with field inocula. To demonstrate the use of this flow system corrosive biofilms were grown and were monitored with confocal microscopy and impedance spectroscopy, scanning electron microscopy.

11) SILVER METAL-ORGANIC-INORGANIC COMPOSITES AS THERMAL INTERFACE MATERIALS

PRESENTER: Nirup Nagabandi, Cengiz Yegin, Jun Kyun Oh and Mustafa AKbulut

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843-3122, U.S.A

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Ever miniaturization of electronic devices with simultaneous increase in computing power is leading to high heat densities and thus failing devices. Effective thermal interface materials are way forward to solve this problem. We developed silver rich composites with thiosemicarbazide functionalized boron nitride nanosheets (f-BNNS) dispersed via electro-deposition process. These composites have high thermal conductivity of 220±10 W/m.K besides having a Youngs modulus of 21±2 GPa. The f-BNNS diffuse in to the electrodepositing matrix via Vander walls interactions and kinetic trapping. f-BNNS which are very close to the electrode kinetically trap in to the copper matrix via Brownian motion. As the particles increase, the vander walls forces dominate according to DLVO theory and diffuse more particles in to the composite matrix. After approaching the silver grains, f-BNNS with functional end group self-assemble via coordination bonding. Changing the functional end group influences the attachment properties and thus the composite itself. Thiol functional group is replaced with cyano and bromo to study the effect of self-assembly strength effect on the composites. Even though the composite construction followed similar mechanism, the thermal conductivity of these composites varied from 220 to 310 W/m.K. with the bond strength while the Youngs modulus remained fairly constant around 21 to 25 GPa. These nano-composites with the high thermal conductivity and low Youngs modulus make an ideal next generation thermal interface material.

12) DYNAMIC MODELING AND OPTIMIZATION OF RENEWABLE HIGH-PRESSURE PEM HYDROGEN PRODUCTION AND STORAGE

PRESENTER: Gerald S. Ogumerem and Efstratios N. Pistikopoulos[1,2]

[1] *Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX*
[2] *Texas A&M Energy Institute, Texas A&M University, College Station, TX*

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Renewable hydrogen production and utilization can be a sustainable path for the stabilization of the power grid. It also provides options for a more amiable evolution of fuel cell vehicles (FCV) to replace fossil-based vehicles. This work presents a systematic approach for modeling and optimization of high-pressure Polymer Electrolyte Membrane (PEM) hydrogen production and Metal Hydride (MH) storage. A detailed mathematical model of a PEM electrolyzer and a MH hydrogen storage system is developed, integrated and validated using experimental data from the literature. The model is optimized to obtain a metal hydride hydrogen storage process design with efficient temperature control to minimize energy usage and storage time. This is done by optimizing the amount of hydrogen stored in the metal hydride within a given time period given material, safety, and operational constraints. This work also illustrates the tradeoff between energy used and the storage time for the hydrogen production and storage.

13) BIG DATA APPROACH TO FAULT DETECTION AND DIAGNOSIS IN BATCH PROCESSES USING NONLINEAR SVM-BASED FEATURE SELECTION

PRESENTER: Melis Onel[1,2], Chris A. Kieslich[1,2], Yannis A. Guzman[1,2,3] and Christodoulos A. Floudas[1,2], Efstratios N. Pistikopoulos[1,2]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

Simultaneous achievement of high process efficiency, safety, and profitability is of utmost importance in modern process industries. A major challenge in industrial applications is the rapid detection and identification of process faults in order to sustain a safe operation and minimize losses in productivity. Statistical process monitoring (SPM) algorithms are often used to detect the deviation from normal operating regimes. A growing number of studies have focused on data-driven process monitoring by using the Tennessee Eastman and Pensim benchmark datasets for continuous and batch processes respectively.

Batch reactor processes are widely used in chemicals, food, and pharmaceutical industry. These processes involve a considerable number of interconnected variables. In addition to inherent non-stationarity, batch processes are characterized with finite duration, nonlinear response, and batch-to-batch variability. High complexity as well as dimensionality of batch processes impose a big challenge in fault diagnosis. Most novel techniques for fault detection and identification have focused on continuous processes, and the need of monitoring algorithm development for batch processes is evident.

We present a new data-driven framework for process monitoring and intervention in batch processes. Central to the framework are novel theoretical and algorithmic developments in support vector machine-based dimensionality reduction which improve accuracy, guide fault diagnosis, and encapsulate highly nonlinear relationships. We will discuss critical data processing and feature extraction steps specific to batch processing. Our methods will be applied to a recent extensive benchmark dataset which features data describing 90,400 batches with numerous and diverse fault types. The analysis framework aims for early detection of faulty batches and enables intervention to reduce loss of profit.

14) STUDY OF FACTORS THAT AFFECT DUST EXPLOSION CHARACTERISTICS OF FIBROUS DUST MATERIALS

PRESENTER: Bharatvaaj Ravi, M. Sam Mannan and Chad Mashuga

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Combustible dust hazard is a serious threat to the process industries. Out of the 281 combustible dust incidents reported by the U.S. Chemical Safety and Health Investigation Board (CSB), 66 incidents have been caused by wood dust. Despite the National Fire Protection Agency's (NFPA) efforts in specifically catering to the wood working and wood-based products manufacturing industries and Occupational Safety and Health Administration's (OSHA) National Emphasis Program on combustible dust hazards, to create awareness and minimize wood dust hazards, the wood dust incidents continue to occur. Since, woody biomass materials are increasingly used as an alternative energy source since last decade the threat to the biomass energy producers due to dust explosion is of great importance. The fundamental difference between traditional dusts and wood dusts is that the latter are flocculent and fibrous. They are not characterized effectively by single linear dimensional descriptor, such as particle diameter, as in the case of traditional – spherical or near spherical – dusts. Various studies in the literature have revealed that the standard dust explosion testing procedures and the categorization of these non-traditional dust based on particle diameter might not be valid. This research explores the effect of particle size and shape definitions, due to differing particle characterization methods, of these fibrous wood dusts on dust explosion behavior. The research tries to simulate the concentration gradient achieved inside a dust explosion using computational fluid dynamics package chamber which is often assumed to be a homogeneous mixture as in a gas explosion. Does the dust concentration give the entire picture of explosion characteristics such as maximum explosion pressure and explosion pressure rise rate? Or

is there a better indicator of these characteristics when it comes to flocculent dust? These are the questions that the current research is trying to answer

15) AN IMPROVED APPROACH FOR ROBUST SCHEDULING UNDER UNCERTAINTY

PRESENTER: Utkarsh D. Shah[1,2], Yannis A. Guzman[3,1,2], Logan R. Matthews[3,1,2] and Christodoulos A. Floudas[1,2]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

In practice, the uncertainty in processing time data frequently affects the feasibility of optimal solution of the nominal production scheduling problem. Using the unit-specific event-based continuous time model for scheduling, we develop a novel multi-stage robust approach with corrective action to ensure robust feasibility of the worst case solution while reducing the conservatism arising from traditional robust optimization approaches. We quantify the probability of constraint satisfaction by using apriori and aposteriori probabilistic bounds for known and unknown uncertainty distributions, consequently, improving the objective value for a given risk scenario. Computational experiments on several examples were carried out to measure the effectiveness of the proposed method. For a given constraint satisfaction probability, the proposed method improves the objective value compared to the traditional robust optimization approaches.

16) HIGH OXYGEN GAS BARRIER IN MULTILAYER THIN FILMS THROUGH PH MANIPULATION OF MONTMORILLONITE CLAY NANOPLATELETS

PRESENTER: Yixuan Song, David A. Hagen and Jaime C. Grunlan

TYPE OF PRESENTATION: ORAL

ABSTRACT:

With a highly ordered nanobrick wall structure, polyelectrolyte-montmorillonite (MMT) clay multilayer nanocoatings can dramatically reduce the oxygen transmission rate (OTR) of polymer films used in various packaging applications (e.g., polyethylene terephthalate (PET) and oriented polypropylene (OPP)) by several orders of magnitude. In an effort to produce high oxygen barrier with fewer deposition steps, pH of the MMT aqueous suspension was reduced. In a polyethylenimine (PEI)/poly(acrylic acid) (PAA)/PEI/MMT quadlayer system, the reduced pH of MMT causes the preceding PEI layer to be more charged, which results in more clay to be deposited per layer. A compromise between high polymer diffusion (high pH) and high clay deposition (low pH) was found at pH 6, where the best oxygen barrier is achieved. A 179 μm thick PET substrate, coated with only three PEI/PAA/PEI/MMT quadlayers (44 nm thick), exhibits an undetectable oxygen transmission rate (< 0.005 cm3/(m2·day·atm)). The calculated oxygen permeability is orders of magnitude below SiOx and metal thin films (<5 ×10-22 cm3·cm/(cm2·s·Pa)). This reduced number of layers necessary for high gas barrier potentially makes these transparent, multilayer thin films interesting for commercial packaging applications.

17) SPRAY-ON POLYMER-CLAY MULTILAYERS AS A SUPERIOR ANTICORROSION METAL PRETREATMENT

PRESENTER: Pilar C. Suarez-Martinez, Jerome Robinson, Hyosung An, Robert C. Nahas, Douglas Cinoman, and, Jodie L. Lutkenhaus

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Pretreatment coatings applied to metals play a very important role in the overall performance of corrosion inhibiting coatings. Hexavalent chromium known for being one of the most used pretreatment for aluminum is now considered harmful. Therefore, a need for environmental friendly yet efficient and scalable pretreatment coatings has emerged. Here, we present the spray-assisted layer-by-layer assembly and anticorrosion performance of a highly ordered clay-polymer nanocomposite coating applied onto aluminum 2024-T3. This approach is an entirely water-based process, allowing for application over large surface areas. This novel pretreatment coating contains 25 wt% clay and presents a brick and mortar multilayered structure, where the montmorillonite clay platelets (MMT) act as a physical barrier for oxygen transport, while also preventing the dissolution of corrosion products – thus slowing the cycle of corrosion. The branched polyethylenimine polymer (BPEI) acts as the mortar and as a proton sponge providing surface buffering once the corrosion process initiates. The anticorrosion properties of the sprayed assisted layer-by-layer assembled coating are evaluated by electrochemical impedance spectroscopy (EIS) and salt spray testing. This BPEI/MMT system presents good anticorrosion properties, which make it an environmentally friendly and scalable alternative pretreatment.

18) ANCHOR-TENANT MODELS FOR THE SYNTHESIS OF ECO-INDUSTRIAL PARKS THROUGH CARBON-HYDROGEN-OXYGEN SYMBIOSIS NETWORKS

PRESENTER: Kevin Topolski[1], Mohamed Noureldin[2], and Mahmoud El-Halwagi[1]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

An eco-industrial park (EIP) is a network of entities who choose to interact by exchanging byproducts, wastes and/or energy to gain benefits greater than unintegrated operations. The concept is particularly attractive for developing industrial clusters and integrating processing facilities within an industrial city.

Recently, the concept of Carbon-Hydrogen-Oxygen Symbiosis Network (CHOSYN) has been introduced for the integration of hydrocarbon processing facilities. The key idea of CHOSYN is to use atomic-level information to set targets for the integration opportunities and to employ a multi-scale systems approach to devising macroscopic strategies to attain the atomic-based benchmarks. CHOSYN takes advantage of the common ground of the chemical industry, utilizing streams containing carbon, oxygen and hydrogen atoms, to create synergism among multiple entities. Optimization approaches and shortcut methods have been developed to synthesize implementation alternatives of a mass integrated network that reduces raw material usage and waste disposal while offering significant economic benefits.

In synthesizing new CHOSYNs or retrofitting an existing system, it is important to account for the various relationships among the EIP participants. The objective of this paper is to adopt the Anchor-Tenant model in the synthesis of CHOSYNs. Anchors are first invited as the key participants in the EIP. “Tenants” are potential plants that could be developed and integrated with the existing “Anchor(s)” thus creating a genesis of an EIP. A multi-scale optimization approach is developed to identify and screen the tenants and to determine performance benchmarks for individual plants and for the whole EIP. Different cooperative and non-cooperative scenarios are examined. The scope is of this study is extended to include nitrogen-based chemistries. A case study is developed and solved to demonstrate the key theoretical concepts and the applicability of the new approach.

19) VERSATILE THERMOCHROMIC SUPRAMOLECULAR MATERIALS BASED ON CHARGE TRANSFER INTERACTIONS

PRESENTER: Tianyu Yuan[1,3], Mariela Vazquez[3], Mark A. Olson[2] and Lei Fang[1,3]

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TYPE OF PRESENTATION: ORAL

ABSTRACT:

Thermochromic materials have attracted many research interests both in and out of academic and industrial circles. Although the phenomena of thermochromism has been commonly observed in inorganic materials, organic thermochromes which can be processed from environmentally friendly solvents are rarely discovered. Herein we report the design and synthesis of a new class of thermochromic supramolecular materials, which can easily be processed from water via a reversible sol–gel transition. The supramolecular materials are composed of a bis-bipyridinium acceptor, a π-electron-rich naphthalene derivative donor, and halogen counterions. Long helical nanofbers can be assembled in water, gelating at room temperature. Inked designs, thin films, and aerogels are solution-processed to exhibit thermochromic behavior based on competing $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ charge transfer interactions. By using different π-electron rich donors, and counterions, we demonstrate that both the color observed at room temperature and at high temperatures can be tailored. The results open up the door to develop novel amphiphile-based thermochromes with water processability and a large tunable color palette.

20) NOVEL JANUS NANOPLATELETS FOR ENHANCED OIL RECOVERY

PRESENTER: Lecheng Zhang, Mingxiang Zeng and Zhengdong Cheng

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: ORAL

ABSTRACT:

Janus nanoplatelets have been observed to have stabling effects on Pickering emulsions. However, existing synthesis methods for Janus nanoplatelets often require complicated procedures and use high-cost templates. Thus, the need for a simpler and more cost efficient way for synthesizing the platelets is eminent. Innovations in asymmetrical surface modifications allows for a more efficient way of producing the Janus nanoplatelets, which can have potential applications in Enhanced Oil Recovery (EOR) for high temperature and high salinity reserviors. The interfacial tension profile and emulsion phase diagram were investigated to compare the quality of nanoplatelets produced using existing methods.

21) SOLID-STATE SYNTHESIS AND THERMOELECTRIC PROPERTIES OF MAGNESIUM SILICIDE

PRESENTER: Azhar Ali[1], Venkata Vasiraju[2], Yixi Chen[1], Sreeram Vaddiraju[1, 2]

[1] *Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station TX 77843*

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Magnesium silicide is an attractive material for thermoelectric applications due to its low toxicity, thermal and mechanical stability, low density, and high relative abundance. However, due to the high vapor pressure of magnesium and its propensity for oxidation, it is often difficult to synthesize large quantities of high quality magnesium silicide using typical melt synthesis techniques. Here, we present a facile, scalable, and reliable technique for the synthesis of pure magnesium silicide from the constituent elemental powders. Solid-state reaction between magnesium and micron-sized silicon particles in a three-zone tube furnace is used to produce the magnesium silicide powder, which is consolidated via hot uniaxial pressing into pellets. X-ray diffractometry (XRD) and Raman spectroscopy confirm the absence of impurities and contaminants in the synthesized magnesium silicide powder. With thermoelectric power factors comparable to those reported in the literature, the synthesized magnesium silicide pellets exhibit promising thermoelectric behavior.

22) GLOBAL OPTIMIZATION OF CONSTRAINED GREY-BOX MODELS FOR WELL INJECTION AND PRODUCTION

PRESENTER: Burcu Beykal[1,2,] Fani Boukouvala[3], Nadav Sorek[4], Hardikkumar Zalavadia[4], Eduardo Gildin[4], Christodoulos A. Floudas[1,2], Efstratios N. Pistikopoulos[1,2]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Waterflooding well-control technology in well injection and production greatly suffers from the curse of dimensionality. Thus, the objective of this study is to introduce a water-control technology based on a new optimization framework that significantly reduces the computational effort for waterflooding well-control optimization problems by (a) reducing the dimensionality of the optimization formulation, and (b) using a constrained grey-box optimization algorithm, which couples deterministic global optimization with surrogate modeling. The first step of this workflow is based on parameterization of the well-control variable domain through a set of functional relationships, which is denoted as Functional Well-Control Method (FCM). Through this approach, we transform the optimization search space from the traditional pressure-based control to a reduced space formed by the coefficients of the selected functional method. These new formulations are then optimized by the ARGONAUT algorithm, which is comprised of several mixed-integer and/or nonlinear optimization sub-problems for (a) sampling selection, (b) surrogate model identification and parameter estimation and, (c) global optimization of the formulated constrained surrogate formulations using the deterministic global optimization solver ANTIGONE. We test the efficiency of the entire framework, with and without constraints, on a realistic three-dimensional reservoir model (UNISIM-I-D Benchmark). Our results demonstrate significant computational savings due to the coupling of ARGONAUT and the FCM formulation. In addition, we compare our results with other gradient-free and gradient-based algorithms which have been traditionally used in the literature (such as NOMAD and EGO) and we demonstrate that our framework leads to improved solutions with higher consistency and with reduced sample-calls to the reservoir simulation.

23) LARGE-SCALE SYNTHESIS OF BYPRODUCT-FREE SEMICONDUCTING NANOMATERIALS: DIRECT CONVERSION OF HIGHLY POROUS ZN PELLETS TO ZN3P2 NANOWIRES

PRESENTER: Yixi Chen, Rakesh Polinnaya, Pranav Kannan, Azhar Ali and Sreeram Vaddiraju

TYPE OF PRESENTATION: POSTER

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

ABSTRACT:

Large-scale synthesis of byproduct-free nanomaterials is one of the major challenges for commercial applications of nanotechnology. For instance, zinc phosphide (Zn3P2) nanowires, which are synthesized on zinc foils and later manually collected from the substrate, contain an appreciable amount of zinc metal when they are consolidated into bulk forms. Herein, a novel approach to synthesizing a large quantity of byproduct-free nanomaterials is proposed, in which highly porous Zn pellets are directly converted to Zn3P2 nanowires. Based on analysis of SEM and XRD, it was confirmed that Zn3P2 nanowires were produced in the whole pellet. This technology can be extended to produce other types of nanomaterials in a byproduct free manner.

24) WATER-BASED ASSEMBLY OF POLYMER-METAL ORGANIC FRAMEWORK (MOF) FUNCTIONAL COATINGS

PRESENTER: Souvik De[1], Manjula I. Nandasiri[2], Herbert T. Schaef[3], Benard Peter McGrail[4], Satish K. Nune[4], and Jodie L. Lutkenhaus[1, 5]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Metal organic frameworks (MOFs) have gained attention for their porosity, size selectivity, and structural diversity. There is a need for MOF-based coatings, particularly in applications such as separations, electronics and energy; yet forming thin, functional, conformal coatings is prohibitive because MOFs exist as a powder. Layer-by-layer assembly, a versatile thin film coating approach, offers a unique solution to this problem, but this approach requires MOFs that are water-dispersible and bear a surface charge. Here, we address these issues by examining water-based dispersions of MIL-101(Cr) that facilitate the formation of robust polymer-MOF hybrid coatings. Specifically, the substrate to be coated is alternately exposed to an aqueous solution of poly(styrene sulfonate) and a MIL-101(Cr) dispersion, yielding linear film growth and coatings with a MOF content as high as 77 wt%. This approach is surface-agnostic, in which the coating is successfully applied to silicon, glass, flexible plastic, and even cotton fabric, conformally coating individual fibers. In contrast, prior attempts at forming MOF-coatings were severely limited to a handful of surfaces, required harsh chemical treatment, and were not conformal. The approach presented here unambiguously confirms that MOFs can be conformally coated onto complex and unusual surfaces, opening the door for a wide variety of applications.

25) SYSTEMATIC PROCESS INTENSIFICATION USING BUILDING BLOCKS

PRESENTER: Salih Emre Demirel, Jianping Li and M. M. Faruque Hasan

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Process intensification combines multiple operations in a single unit, and leads to substantially smaller, cleaner, safer, and more energy-efficient technologies. Current superstructure-based process synthesis relies on pre-specified equipment configurations which hinders automatic identification of intensified equipment configurations. Phenomena based process intensification, allows to approach processes from a lower aggregation level which enables identification, screening and incorporation of intensification opportunities, but this approach often requires sequential or decomposition based solution strategies to solve large models, which can lead to suboptimal solutions. In this work, a unified process synthesis and intensification method that utilizes an original building block-based superstructure is proposed. Proposed superstructure is an ensemble of building blocks, where each block represents a unit use of a material. Nexus between the blocks are achieved via intra-block streams. An intensified unit is realized by selecting and assembling multiple neighboring blocks with different functionalities. This enables to incorporate many intensification alternatives, including divided wall column distillation, reactive distillation, reactive absorption and membrane reactor, within the same superstructure without any a priori postulation. The overall process intensification model is formulated as a single mixed-integer nonlinear optimization (MINLP). Hence, given feed and product

specifications and available materials, building block-based superstructure is able to generate intensified process flowsheets with optimum operating conditions.

26) IMPROVED DATA-DRIVEN MATHEMATICAL MODELING AND GLOBAL OPTIMIZATION FRAMEWORK: AN APPLICATION IN REFINERY PLANNING OPERATIONS

PRESENTER: C. Doga Demirhan[1,2], Fani Boukouvala[1,2,3], Kyungwon Kim[4], Hyeju Song[2], Efstratios N. Pistikopoulos[1,2] and Christodoulos A. Floudas[1,2]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Improving the planning and scheduling operations is one of the major challenges in the petrochemical industry considering the tight competition, environmental regulations, and lower profit margins. A recent work of our group developed a data-driven modeling and global optimization-based planning formulation for highly integrated refinery-petrochemical complexes. In this work, an improved and generalized framework for planning operations is applied to an actual refinery operated by Hyundai Oilbank and located in Korea.

The refinery planning problem has received considerable attention and it is a topic of special interest for many process systems engineers and in this respect, nonlinear models and specialized algorithms have been proposed for refinery operation but global optimality was not guaranteed in any method. Data-driven input-output models offer a promising way to obtain inexpensive nonlinear models as opposed to computationally expensive commercial processing unit models.

In the first step of this work the raw data provided by the industrial partner are organized, analyzed, and processed. Then, data-driven nonlinear models are developed for the processing units. The primary approach is to use quadratic, bilinear, and linear models to predict product yields and properties for all of the production units. The parameters of the postulated models are globally optimized using the state-of-the-art, commercial deterministic global optimization solver ANTIGONE. All the models are created in a generalized and an automated fashion.

In the second step a superstructure containing all possible connections and operating modes in the refinery is created. The resulting single-period planning model is a large-scale non-convex mixed integer nonlinear optimization model, which is solved to ε-global optimality using ANTIGONE.

Results of several case studies illustrate the efficiency of our proposed model and global optimization approach.

27) MONETIZATION OF STRANDED GAS THROUGH AMMONIA AND UREA PRODUCTION

PRESENTER: Zehao Gou, Debalina Sengupta, Mike Dou and M.M. El-Halwagi

TYPE OF PRESENTATION: POSTER

ABSTRACT:

The world demand for total fertilizer nutrients will reach 200 million metric tons in 2018. In the meantime, 6.3 trillion cubic feet per year natural gas are vented, flared and reinjected worldwide. Ammonia and urea production are promising routes to monetize these stranded gas resources. Greenhouse gas reduction through the incorporation of CO2 generated in the reforming section into urea production is a plus for this process. This study examines and optimizes the ammonia and urea processes by techno-economic analysis, safety analysis, process intensification and

heat integration. A case study is carried out on deploying the technology in Indiana (a state with a thriving agricultural sector and heavy demand for fertilizers). A medium gas reserve size of 10 MM SCFD is chosen to maintain the flexibility of the process. The process includes a reforming section, high-temperature shift, low-temperature shift, CO2 recovery, methanation, ammonia synthesis, refrigeration, ammonium carbamate condensation, urea generation and gas recycle. Kinetic models are used to set the rate while equilibrium criteria are chosen to build the boundary in this simulation. Two process intensifications – autothermal reforming and combi- reactor – are proposed to increase the mobility of the system. Heat integration is carried out to minimize the usage of external heating and cooling utilities.ver miniaturization of electronic devices with simultaneous increase in computing power is leading to high heat densities and thus failing devices. Effective thermal interface materials are way forward to solve this problem. We developed silver rich composites with thiosemicarbazide functionalized boron nitride nanosheets (f-BNNS) dispersed via electro-deposition process. These composites have high thermal conductivity of 220±10 W/m.K besides having a Youngs modulus of 21±2 GPa. The f-BNNS diffuse in to the electrodepositing matrix via Vander walls interactions and kinetic trapping. f-BNNS which are very close to the electrode kinetically trap in to the copper matrix via Brownian motion. As the particles increase, the vander walls forces dominate according to DLVO theory and diffuse more particles in to the composite matrix. After approaching the silver grains, f-BNNS with functional end group self-assemble via coordination bonding. Changing the functional end group influences the attachment properties and thus the composite itself. Thiol functional group is replaced with cyano and bromo to study the effect of self-assembly strength effect on the composites. Even though the composite construction followed similar mechanism, the thermal conductivity of these composites varied from 220 to 310 W/m.K. with the bond strength while the Youngs modulus remained fairly constant around 21 to 25 GPa. These nano-composites with the high thermal conductivity and low Youngs modulus make an ideal next generation thermal interface material.

28) LIQUID SURFACTANTS FOR PROCESSING BORON NITRIDE NANOSHEETS (BNNSS)

PRESENTER: Touseef Habib[1], Dinesh Sundaravadivelu Devarajan[2], Fardin Khabaz[2], Dorsa Parviz[2], Thomas C. Achee[2], Rajesh Khare[2] and Micah J. Green[1]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Boron nitride nanosheets (BNNSs) are a tremendous nanomaterial with excellent material properties, but obtaining them through liquid-phase exfoliation remains challenging due to low yields in common solvents. Recent studies suggest co-solvent mixtures or mixtures of alcohol and water at certain weight ratios can yield BNNSs dispersions with a higher concentration. The role of alcohols, specifically the role of t-butanol for BNNSs stability in dispersions will be explained. Through carefully crafted experiments and with molecular dynamics simulations, it was established that t-butanol behaves like a liquid dispersant; interacting with both water molecules and nanosheets to prevent aggregation. The BNNSs obtained from these dispersions are not only of high quality (as shown by TEM images), but the dispersions can also be freeze dried to obtain non-aggregated BNNSs powder. The freeze dried BNNSs powder are re-dispersible without the need of any additional exfoliation steps; the freeze dried BNNSs powder can be utilized in different industrial processes (from coatings to polymer fillers) without the worry of aggregation.

29) BIODEGRADABLE 3D PRINTED OIL ABSORBENTS WITH TUNABLE CAPILLARY ARCHITECTURES

PRESENTER: Duanduan Han and Victor Ugaz

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Here we show how 3D printing can be leveraged to manufacture absorbents with tailored internal oleophilic capillary networks capable of selectively extracting and sequestering oil dispersed in water. These networks are produced using poly(lactic acid), an inexpensive commodity biopolymer that is degradable and environmentally friendly. 3D printing enables designer absorbent architectures to be crafted that match properties of different petroleum fractions, maximize selectivity against water, and permit either strong encapsulation or easy recovery of the collected oil. We describe fundamental characterization studies aimed at identifying optimal pore network architectures that maximize uptake and rate of absorbance, as well as determining quantitative cost/performance metrics for rational selection of optimal designs. This platform lays a foundation to manufacture a host of products incorporating sophisticated oil absorption and encapsulation functions. We demonstrate this versatility by highlighting two innovative applications. First, we demonstrate the ability to produce large-sized 3D printed absorbent filters that can be incorporated into an autonomous robotic oil skimmer, enabling continuous routine clean-up of waterways. 3D printing makes it possible to overcome the limitations of current sheet or pad-based materials by achieving on-demand rapid production of rugged, reusable, rigid absorbents with superior uptake, selectivity, and ease of deployment. Second, we employ a new family of flexible filaments to produce 3D printed wearable products containing embedded capillary networks tailored to encapsulate oil-based insect repellents. A core-shell design is embedded in a wristband format to uniquely deliver sustained release of dispersed volatile species at higher doses than possible when applied directly to the skin. This approach may offer a new avenue to help combat the spread of mosquito-borne infectious disease.

30) DUST-GAS HYBRID MINIMUM IGNITION ENERGY PREDICTION

PRESENTER: Haitian Han and Chad V. Mashuga

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

A large percentage of the raw materials, intermediates and finished products in the chemical process industry are solids. Processing of the solids often results in dusts which when suspended in air have the potential to result in a deflagration if the concentration is adequate and a minimum amount of ignition energy is present (MIE). This situation becomes more complex when a flammable gas or vapor is present along with the dust, resulting in a hybrid system. The hybrid minimum ignition energy (HMIE) is the smallest amount of energy required to ignite a dust/gas system. There is limited understanding of the interactions between combustible dust and flammable gas during the ignition process. Models to predict the HMIE are limited in literature. The objective of the current research is to study the fundamental contributions of the hybrid flammable dust/gas systems for various families of materials to develop better prediction models. Meanwhile, a new method by purging the Hartmann tube is applied prior to ignition in order to improve a more conservative procedure to test HMIE.

31) RAPID MICROWAVE-ASSISTED SYNTHESIS OF HYBRID ZEOLITIC-IMIDAZOLATE FRAMEWORKS WITH MIXED METALS AND MIXED LINKERS

PRESENTER: Febrian Hillman[1], John Zimmerman[1], Seung-Min Paek[3], Mohamad R. A. Hamid[1], Woo T. Lim[4] and Hae-Kwon Jeong*[1,2]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Separating a crude component into a more valuable purer product is a major part of many industrial chemical plants. Typically these processes utilize distillation, which account to 10 – 15 % of world's energy consumption. One alternative solution that can reduce energy consumption is through membrane separation using porous solid material such as metal organic frameworks (MOFs). Zeolitic-imidazolate frameworks (ZIFs), a subclass of MOFs, in particular have attracted many attentions due to their chemical/thermal stabilities, their ultra-miroporosities, and high surface area when compared to other MOFs material. ZIFs are frameworks consisting transition metals bridged by imidazolate-derived ligands. A common drawback for membrane gas separation is the limited availability of pore size and functionalities. Studies have shown that through mixing metals and ligands, one can continuously tune the ZIFs (termed hybrid ZIFs) properties to match with the characteristic of specific gas mixture. However, The common synthesis of hybrid ZIFs has generally been through slow conventional solvothermal methods, requiring several hours up to days, which can be an economical issue for hybrid ZIFs to be used in a large industrial scale.

Herein we report a new microwave-assisted (MW) synthetic strategy to rapidly prepare hybrid ZIFs with mixed metal centers and/or linkers. The MW method significantly shortens synthesis time, produces higher yield, substantially reduces the amount of ligand, and eliminates the use of deprotonating agents. Several characterizations were performed to determine the structure and properties of the hybrid ZIFs. Furthermore, for the first time, a hybrid ZIF with both mixed metal centers and mixed linkers was prepared through one-step microwave synthesis. Finally, a mixed metal CoZn-ZIF-8 was grown as membranes, showing higher propylene/propane separation factor (~120) when compared to pure Zn-ZIF-8 membranes (~63) prepared with similar method.

32) USING BLACK PARTICLES AS AN ADDITIVE TO PRODUCE TUNABLE STRUCTURAL COLORS WITH HIGH COLOR CONTRAST IN PHOTONIC CRYSTALS

PRESENTER: Dali Huang, Minxiang Zeng, Lecheng Zhang and Zhengdong Cheng

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station TX 77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

The structure color of photonic crystal has been attracting remarkably interest. Man-made polystyrene photonic crystal has a general milky white looking whose structural colors are faint and need improving. The color enhanced PS hybrid photonic crystals were designed and fabricated through introducing a new type of graphene quantum dot. The visual appearance of colloidal crystal coatings changed markedly from faint milky white to brilliant colors after doping GQDs and can be tuned through concentrations of GQDs in the photonic crystal.

33) ELECTROLYTE STRUCTURE AND BEHAVIOR OF POLYSULFIDE SPECIES IN LITHIUM-SULFUR BATTERIES

PRESENTER: Ethan P. Kamphaus[1], Perla B. Balbuena[1,2]

[1] *Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843*

[2] *Texas A&M University, Department of Materials Science and Engineering*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Batteries with large amount of energy storage are needed to meet the requirements of modern technology and electronics like electric vehicles or cell phones. Current lithium ion batteries are unable to meet these modern energy demands; new battery technology is required. The lithium-sulfur (Li-S) battery is promising technology that has the theoretical energy capacity to meet societal needs. However, several large issues plague Li-S battery performance such as the polysulfide shuttle reaction which results from migration to the anode side of soluble Li polysulfide species formed at the cathode surface. The dissolution of polysulfide species in the electrolyte is the fundamental issue driving this parasitic shuttle reaction. However, the solvation structure and fundamentals are not well known due to the

complex interactions and chemistry in Li-S batteries. The molecular processes are difficult to study experimentally and therefore are not well understood.

Quantum scale density functional theory (DFT) and ab-initio molecular dynamics (AIMD) were used to investigate and screen different electrolyte compositions in order to identify the structure and behavior of lithium and polysulfide solvation. Promising and interesting electrolytes interactions can be identified by computational simulations to help with experimental design of batteries. Electrolytes consisting of Dimethoxyethane, Dioxolane, and fluorinated ethers in the presence of lithium salts were investigated. We gained a better fundamental understanding polysulfide's solvation and behavior in electrolyte and established the basis for a rational design that may improve overall Li-S battery performance by reducing the shuttle redox reaction.

34) SIMULTANEOUS DESIGN AND CONTROL OF A BINARY DISTILLATION COLUMN

PRESENTER: Baris Burnak, Justin Katz, Nikolaos A. Diangelakis and Efstratios N. Pistikopoulos

Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Simultaneous strategies for process and control design are expected to deliver integrated and intensified processes with reduces costs and energy requirements [1]. In this study, we present a systematic framework for the simultaneous design and control of a binary distillation column. Based on our recently introduced PAROC framework [2] the proposed strategy features: (i) a high-fidelity model implemented in gPROMS ®, (ii) a model reduction step, through MATLAB ® system identification toolbox (iii) a multiparametric optimization and explicit model predictive control step (POP) [2] for the design of a MIMO (multiple input - multiple output) system, with the pressure and reflux ratio as the manipulated variables and the distillate and bottom product composition as the control variables, (iv) a closed loop validation step against the high-fidelity model. Both continuous (column diameter, condenser and reboiler area) and binary variables (reflux and feed tray location) are considered. Comparison of the simultaneous strategy versus a sequential design procedure is also presented, demonstrating distinct benefits of the integrated approach.

35) MODELING LPS-INDUCED TNF-A PRODUCTION IN MACROPHAGES

PRESENTER: Dongheon Lee[1,2], Yufang Ding[3], Arul Jayaraman[1,3], and Joseph Sangil Kwon[1,2]

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[3] *Department of Biomedical Engineering, Texas A&M University, College Station, TX*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Macrophages are ubiquitous throughout the body and involved in various physiological responses. Namely, macrophages are indispensable in innate and adaptive immune responses . Such immune responses are mediated by its membrane receptors by recognizing pathogens and pathogen-derived molecules. Macrophages express Toll-like receptor 4 (TLR4), and TLR4 can recognize LPS (lipopolysaccharide), which is a major component of bacterial outer membranes . Recognition of LPS by TLR4 initiates intracellular signaling pathways and downstream gene expression to rapidly eliminate the bacterial components. As a result, transcription factor NF-κB is activated, which leads to the production of the pro-inflammatory cytokine TNF-α (tumor necrosis factor-α). TNF-α, in turn, initiates signaling through the TNF signaling pathway and propagates the inflammatory response. Hence, LPS-induced signaling pathway is an important part of the early immune response.

Previous studies have constructed population-level models to study the dynamics of signaling through the NF-κB pathway. Predictions from the population-level model could be misleading since the model masks the behaviors of individual cells. It has been shown that the effect of LPS stimulation can be highly heterogeneous across the population. Therefore, we attempted to develop a stochastic model of LPS-induced NF-κB signaling and TNF-α production in macrophages. Specifically, enzymes and proteins involved were modeled as states, and the corresponding kinetic parameters for intracellular signaling pathway were identified via inverse modeling. In order to validate model

predictions, the activation of TNF-α and IκB in RAW macrophages under different LPS doses was quantified using flow cytometry and intracellular staining at the single-cell level. The model is expected to predict the diversity of cellular responses that cannot be captured by deterministic and population-based models. Furthermore, it was possible to simulate intercellular interactions with this stochastic model to analyze cell-to-cell communications - a step toward constructing the multicellular or tissue model.

36) SIMULTANEOUS PROCESS NETWORK SYNTHESIS AND PROCESS INTENSIFICATION USING GRID SUPERSTRUCTURE

PRESENTER: Jianping Li, Salih Emre Demirel and M. M. Faruque Hasan

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Process synthesis is used in obtaining the best processing route among many alternatives by assembling units into a process network with the goal of optimizing either economic, environmental, and/or social objectives [1-2]. Current optimization-based process synthesis methods are unable to automatically construct and identify novel intensified equipments as they require pre-specified equipment configurations. Furthermore, whenever a new problem is addressed, a different superstructure needs to be postulated. To address these challenges, we propose a new building-block based superstructure instead of classical unit-operation based one [3]. Each block represents a unit use of materials with a specific function (reaction, separation, storage). An assembly of the same blocks results in a classical unit operation, while intensified units are realized with assembly of multiple different blocks. This allows a systematic identification, representation and generation of intensification alternatives at the flowsheet level without a priori postulation of their existence. The proposed approach not only identifies different process equipment, but also automatically generates the corresponding flowsheet. We pose the unified synthesis and intensification problem as a mixed-integer nonlinear optimization (MINLP) problem. The objective is to synthesize a process with intensified units by minimizing or maximizing a process metric given the feed and product specifications, feed and product prices, material properties and bounds on flow rates. We also demonstrate that the simultaneous synthesis and intensification approach leads to substantially smaller, cleaner, safer, and more energy-efficient designs.

37) COUNTERCURRENT ENZYMATIC SACCHARIFICATION AND CONTINUUM PARTICLE DISTRIBUTION MODEL OF PRETREATED CORN STOVER

PRESENTER: Chao Liang, Mark Holtzapple and M. Nazmul Karim

Artie McFerrin Dept. of Chemical Engineering, Texas A&M University, College Station TX 77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Enzymes are a major cost contributor in biofuel production using the sugar platform. Conventionally, enzymatic saccharification is performed in batch. A new continuous countercurrent method is explored to more efficiently use enzymes.

In our experiments, batch saccharification was performed on lime + shock pretreated corn stover at various enzyme loadings and reaction times. The HCH-1 Model was utilized to validate experimental results. Countercurrent saccharification was performed on the same substrate at enzyme loadings CTec3 (1 mg protein/g dry biomass), CTec3 (1 mg protein/g dry biomass) + HTec3 (1 mg protein/g dry biomass), and CTec3 (2 mg protein/g dry biomass) + HTec3 (2 mg protein/g dry biomass). To reach a given glucan conversion at low enzyme loadings, countercurrent saccharification reduced enzyme loadings by 1.9 times compared with batch saccharification but was not helpful at high enzyme loadings. The Continuum Particle Distribution Model (CPDM) was used to validate the experimental results and predict sugar yields at various reaction conditions, such as enzyme addition locations, enzyme loading rates, and volatile solid loading rates.

38) COMPUTATIONAL STUDY OF THE ADSORPTION OF A PHENANTHRENE DERIVATIVE OVER A MODEL ZEOLITE

PRESENTER: Monica M. Garnica-Mantilla[1,2], Ana E. Torres-Hernández[1], Luis E. Camacho-Forero [1], Carlos M. Celis-Cornejo[2], Gustavo E. Ramírez-Caballero[2] and Perla B. Balbuena[1]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Petroleum industry processes need to be constantly updated due to significant changes in the physicochemical properties of the oil reserves. For instance, hydrocracking is a viable catalytic process used in conventional refineries that transforms heavy crude oil into desired liquid products. Theoretical and experimental studies have been carried out aiming to understand the stages taking place during this process. Common feedstock, such as vacuum gas oil is composed of polycyclic aromatic hydrocarbons (PAHs) and high concentrations of heteroatom-based compounds. The presence of the latter, even in low amounts, reduces the selectivity and conversion of the process. Common catalysts used in this process are composed of active metals like NiMo, NiW, Pd or Pt supported over amorphous aluminosilicates or zeolites. On the other hand, it has been proposed that the hydrocracking catalysts such as NiMo/ H-Y zeolites are bifunctional. PAHs are partially hydrogenated by the metal while isomerization, ring opening, and dealkylation take place in the porous support. In this work, the hydrocracking reaction is studied using Density Functional Theory (DFT) calculations. The partially hydrogenated phenanthrene-like product reacts at the acid site of a model mordenite zeolite. The geometry of the minima and transition structures along the reaction pathway are optimized at m062x/6-311G(d,p) level of theory and its nature was verified through frequency calculations. Intrinsic Reaction Coordinate (IRC) calculations are performed in order to verify the connectivity of the transition states with the reactants and products. It was found that the electrostatic adducts which resemble ion-pair complexes, detected for zeolite catalysts, could play an important role to enable the reaction to proceed through an energy-favorable channel and could explain its selectivity.

39) ELECTRIC FIELD INDUCED BIREFRINGENCE IN ISOTROPIC SUSPENSIONS OF NANOPLATES

PRESENTER: Carlos Mejia[1], Abhijeet Shinde[1], Ivan Dozov[4], Padetha Tin[5], Patrick Davidson[4], and Zhengdong Cheng*[1,2,3]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Colloidal nanoplates are emerging materials for electronic display applications. It is very imperative to measure the induced-birefringence and Kerr effect of our suspension, α-zirconium phosphate, to have a better understanding of their electro-optical properties. We tested the electric field induced-birefringence in isotropic suspensions of nanoplates with uniform thickness and high diameter to thickness ratio which were varied between 600 to 1200. The systematic variation in aspect ratio allowed us to study the dependence of Kerr coefficient on nanoplate dimensions which follows the Maxwell-Wagner-O'Konski (MWO) model. Kerr coefficient of α-ZrP nanoplates is higher than other platelet systems such as gibbsite, beidellite but lower than graphene oxide.

40) MODEL ORDER REDUCTION OF PARABOLIC PDE SYSTEMS BASED ON TEMPORALLY-LOCAL DYNAMIC MODE DECOMPOSITION WITH CONTROL

PRESENTER: Abhinav Narasingam and Joseph Sang-Il Kwon

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station TX 77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

More often than not a chemical process can be accurately described using a mathematical model which is generally comprised of nonlinear partial differential equations (PDE). In order to accurately capture the dynamics of systems described by PDEs, a large number of state variables are required and this makes it computationally expensive to design online control strategies. Dynamic Mode decomposition with control (DMDc) is an effective model reduction technique that has been developed by the fluids community to analyze observational data arising from high-dimensional dynamic systems that require control. It is a data driven, equation free architecture that approximates the underlying dynamics from snapshot measurements alone. However, the dimension of the reduced order model is often higher than what is required for the design of real-time feedback control systems. Motivated by this consideration, we present a temporally-local model order-reduction technique for nonlinear parabolic partial differential equation (PDE) systems. Specifically, we derive low-dimensional models that approximate the original solution by constructing appropriate temporally-local dynamic modes. Within this context, we partition the time domain into multiple clusters using the global optimum search (GOS) optimization framework, by formulating the clustering problem as a Mixed-Integer Nonlinear Programming problem. We solve the MINLP by decomposing it into a primal problem (LP) and a master problem (MILP). Following the cluster generation, local modes are constructed by applying DMDc to the snapshots contained within each cluster. These dynamic modes are subsequently used as basis functions to compute approximate solutions to the original PDE system. The proposed technique is applied to the incompressible Newtonian fluid flows described by the one dimensional Burgers' equation with distributed control.

41) A NEW SEMI-AUTOMATED HAZID METHOD FOR MORE COMPREHENSIVE IDENTIFICATION OF HAZARDOUS SCENARIOS

PRESENTER: Sunhwa Park, Yan-Ru Lin, and M. Sam Mannan

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering Texas A&M University, College Station TX 77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Despite the substantial development of HAZID methods, traditional HAZID tools still need further development because of their weaknesses in identifying possible hazards; continual catastrophic events occur even after reviewing potential scenarios with HAZID tools. Therefore, it is evident that the unintended incidents that occasionally occur in the chemical process industry require more enhanced HAZID methodologies. With this new HAZID methodology, this study seeks to identify possible scenarios with a semi-automatic and systemic approach. Based on the two traditional HAZID tools, Hazard Operability (HAZOP) Study and Failure Modes, Effects, and Criticality Analysis (FMECA), the new method will minimize the limitations of each method. Additionally, rather than depending on the HAZID tools to achieve the connectivity of the process system, this study will consider the connection with other new technologies in advance. Then, this method can be integrated with proper guidelines regarding process design and safety analysis. To examine its usefulness, the method will be applied to a case study and its outcome will be compared with the actual result, performed before by a traditional HAZOP meeting.

42) ARAMID NANOFIBER/GRAPHENE/CARBON NANOTUBE COMPOSITE ELECTRODES FOR STRUCTURAL ENERGY AND POWER

PRESENTER: Anish Patel [1], John Harris[1], and Jodie L. Lutkenhaus[1,2]

[1]*Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station TX 77843*

[2] *Department of Materials Science and Engineering, Texas A&M University*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Multifunctional energy storage devices can greatly impact public safety and flexible electronics. Mechanically strong energy devices could prevent catastrophic failure in batteries or act as structural elements, simultaneously dissipating energy and bearing a load. While much research has gone into improving the energy storage capabilities of promising materials such as reduced graphene oxide, less attention is paid towards its mechanical properties. Herein we report on multifunctional composite electrodes, consisting of graphene, aramid nanofibers (ANFs), and carbon nanotubes (CNTs), made via flow-directed assembly, and the improvement in mechanical and electrochemical performance due to the incorporation of CNTs.

43) THE PRODUCTION OF HIGH-VALUE INTRACELLULAR COMPOUNDS USING A PROCESS SYNTHESIS FRAMEWORK

PRESENTER: Alexander M. Sabol[1], Maria-Ona Bertran[2], Jonathan P. Raftery[1], John M. Woodley[2], Rafiqul Gani[2], M. Nazmul Karim[1]

[1] *Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station TX 77843*

[2] *Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Systematic process synthesis approaches are widely applied to traditional chemical process industries, but have seen limited use in the bioprocessing industry due to little or no thermodynamic or kinetic data is available. In this work, the process synthesis problem for the bio-manufacturing of high-value intracellular compounds is addressed using a systematic framework that allows for the user to input key process parameters. The framework is based on a superstructure optimization approach and integrates various methods and tools, including a generic model and a database for data management. The framework is implemented in Super-O, a software which guides the user through the formulation and solution of synthesis problems following three steps: (1) problem definition, (2) superstructure generation and data collection, and (3) solution of the optimization problem.

The generic process model consists of a series of processing tasks, namely mixing, reaction, waste removal and product separation, for which the model parameters need to be provided by the user. However, the limited availability of technology data for bioprocesses is a bottleneck in the superstructure development. The experimental values are used to complement data available in the literature and from simulations.

As a case study to exemplify this framework, the production of β-carotene from recombinant Saccharomyces cerevisiae (SM14) consuming glucose via cultivation is analyzed. Processing alternatives are represented in a superstructure, which is the input to Super-O. The first processing step is based on previous studies using SM14. Five recovery steps and two purification steps are also considered in this work, with multiple alternatives for each of them. The optimal process topology for the β-carotene production process has been posed as a profit maximization problem, including OPEX and CAPEX, where given the raw material and product, the optimal process topology is determined.

44) TEMPLATE-FREE 3D TITANIUM CARBIDE (MXENE) PARTICLES CRUMPLED BY CAPILLARY FORCES

PRESENTER: Smit. A. Shah, T. Habib, H. Gao, P. Gao, W. Sun, M. J. Green and M. Radovic

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

MXenes are a relatively new class of nanosheets and they have gained significant interest due to their unique chemical, dielectric and transport properties. Since their discovery in 2011, they have been shown to be promising in

range of applications such as batteries, supercapacitors, electromagnetic shielding, and water desalination. There was a lack of research on changing the morphology of these nanosheets which might potentially open doors to many new fascinating applications. In this study, we have shown that Ti3C2 MXenes can be reversibly processed into a 3D crumpled structure. This was achieved by using capillary forces of a drying droplet in a commonly used industrial spray dryer. Without using any template, we were able to obtain scrolled, bent and folded 3D structures and the morphological change was found to be reversible upon rehydration. We also showed that the extent of crumpling can be controlled by adjusting the spray drying parameters.

45) MODELING OF HYDRAULIC FRACTURING AND DESIGN OF ONLINE OPTIMAL PUMPING SCHEDULE TO ACHIEVE UNIFORM PROPPANT CONCENTRATION

PRESENTER: Prashanth Siddhamshetty[1,2] and Joseph Sangil Kwona[1,2]

[1] *Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843*

[2] *Texas A&M Energy Institute, Texas A&M University, College Station, TX 77845*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

From a control engineering viewpoint, hydraulic fracturing has been traditionally viewed as an open-loop problem. Typically, well logs and mini-frac test results are interpreted prior to operation in order to obtain petrophysical and rock-mechanical properties of the formation. Then, a pumping schedule is designed offline based on the measured properties and applied to a hydraulic fracturing process. However, such an open-loop operation may lead to poor performance, which has motivated this work that considers the closed-loop operation of a hydraulic fracturing process. Initially, we focus on the development of a first-principle model of a hydraulic fracturing process. Second, a novel numerical scheme is developed to deal with the high computational requirement caused by coupling of multiple partial differential equations (PDEs) defined over a time-dependent spatial domain. Third, a reduced-order model (ROM) is constructed, which is used to design a Kalman filter to accurately estimate unmeasurable states as well as to effectively handle the process and measurement noise. Lastly, model predictive control (MPC) theory is applied for the design of a feedback control system to achieve uniform proppant concentration across the fracture at the end of pumping. We demonstrate that the proposed control scheme is able to generate a spatial concentration profile which is closer to the target concentration compared to that of the benchmark, Nolte's pumping schedule. This is because the proposed control system makes use of the real-time measurements as a feedback by taking into account practical considerations such as a) the fact that a pumping schedule consists of multiple stages where the concentration at each state remain constant, b) the desired fracture geometry that has to be satisfied at the end of pumping to maximize the productivity of a fractured well for a given amount of proppant to be injected, and c) state and inputs constraints to prevent early-termination of the hydraulic fracturing process.

46) BINDING OF CHOLERA TOXIN SUBUNIT B WITH HETEROGENEOUS GLYCOLIPIDS ON CELL MIMICKING SURFACES

PRESENTER: Pratik Krishnan, Akshi Singla, Chin-An Lee, Joshua D. Weatherston, Nolan C. Worstell, and Hung-Jen Wu

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station TX 77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

GM_1 has generally been considered as the major receptor that binds to cholera toxin subunit B (CTB) due to its low dissociation constant. However, using a unique nanocube sensor, we have shown that CTB can also bind to other glycolipid receptors, fucosyl-GM_1 (fGM_1) and GD_1b, and in fact with a higher binding capacity than GM_1. Additionally, we have demonstrated that GM_2 can also contribute to CTB binding if present in a glycolipid mixture with a strongly binding receptor (GM_1/fucosyl-GM_1 /GD_1b). This hetero-multivalent binding result was unintuitive because the interaction between CTB and pure GM_2 is negligible. We hypothesized that the reduced dimensionality of

CTB-GM_2 binding events is a major cause of the observed CTB binding enhancement. To test this hypothesis, we altered the surface reaction rate by modulating the fluidity and heterogeneity of the model membrane. Decreasing membrane fluidity reduced the binding cooperativity between GM_2 and a strong receptor. Our findings indicated that a new protein-receptor binding assay, that can mimic complex cell membrane environment more accurately, is required to explore the inherent hetero-multivalency. We have thus developed a new membrane perturbation protocol to efficiently screen receptor candidates involved in hetero-multivalent protein binding.

47) INCORPORATING HUMAN FACTORS ENGINEERING METHODS IN THE SYSTEM LIFE CYCLE OF OFFSHORE OIL AND GAS INDUSTRIES

PRESENTER: Changwon Son, Syeda Zohra Halim, Yogesh Koirala and M. Sam Mannan

Mary Kay O'Connor Process Safety Center

TYPE OF PRESENTATION: POSTER

ABSTRACT:

This paper highlights the importance of integration of human factors engineering (HFE) principles throughout phases of system life cycle of offshore energy industries. Human error is found to be the most common cause of offshore incidents according to the analysis of BSEE incident data. While human operators are mostly blamed for making errors and mistakes at the sharp end of a system, accident models and systems theory tell us that the cause of incidents are triggered much earlier in the system life cycle by the blunt end or managers and designers. Therefore, this proceeding provides HFE considerations for each step in system life as well as available HFE tools and methods to be employed. For corporate organizations to buy in proposed HFE methods, meta-analysis of cost-effectiveness for early HFE implementation is briefly presented.

48) THE INTEGRATION OF DESIGN, CONTROL, AND SAFETY

PRESENTER: Denis Su-Feher, Yogesh Koirala, Efstratios Pistikopoulos and M. Sam Mannan

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Current inherently safer design strategies in the conceptual design stage focus on reducing the overall hazard of a process plant without considering the operability of the process. The process is first designed to be inherently safer with respect to a nominal, steady-state case. Then, after the process is designed, layers of protection are added and operability issues are addressed. However, this sequential design approach does not account for the impact of the design itself on the operability of the facility. A particular design may be safer with respect to its steady-state operation, but may suffer from operability issues. For example, an intensified process may contain less of a hazardous substance and thus be inherently less hazardous, but the design may restrict the controllability of the process, thus making the design have a higher risk and be more prone to loss. A considerable depth of research has been done to simultaneously optimize the design and control system of process plants, but no such approach has integrated inherent safety, only seeking to produce an economically optimal design rather than a safer one.

The objective of this research is to implement a strategy to simultaneously design and control an inherently safer plant. The Parametric Optimization and Control (PAROC) framework will be used as a case study to show how the simultaneous inherently safer design of the plant and the controller can be implemented.

An extensive literature review identified metrics by which controllability of a process plant can be identified and optimized along with the design, as well as inherently safer design indices that can be implemented into the PAROC framework. These metrics and inherently safer design indices will be compared to create a new index for the integration of inherently safer design and control.

With process systems and their dynamics becoming increasingly complex, consideration of operability issues in the design stage becomes even more necessary to prevent incidents. The integration of inherently safer design and control will substantially reduce operability issues that result from an uncontrollable process design and allow for greater tolerance and ease of control.

49) SYNTHESIS AND CHARACTERIZATION OF CDIF-1: A CADMIUM VERSION OF ZIF-8

PRESENTER: Jingze Sun[1], Liya Semenchenko[2], and Hae-Kwon Jeong[1, 3]

[1] *Artie McFerrin Department of Chemical Engineering and 3Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843*

[2] *The Department of Chemical Engineering at the University of Florida, 1030 Center Drive, Gainesville, FL 32611*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Metal organic frameworks (MOFs) are comprised of inorganic nodes and organic ligands as linkers, exhibiting well-defined crystalline structure as well as high porosity. Zeolitic-imidazolate frameworks (ZIFs) are a subclass of MOF. By sharing the same bond angle as the T-O-T bond in zeolites, ZIFs share zeolite topologies as well. Structures of zeolites can be used to describe to the corresponding structure of ZIFs

Comparing to the energy-intensive cryogenic distillation, membrane separations for light hydrocarbons is a novel promising green separation methods. However, light hydrocarbons have a large variety of molecular sizes caused by the difference in the number of carbons, the degree of unsaturation and the existence of isomer. This may require various MOF materials as molecular sieves for them, while in reality, the number of existing ZIF polycrystalline-membrane materials are not as much. To extent the application of membrane separation for light hydrocarbons, new membrane materials will be helpful.

Here we report first methanol-based recipe for synthesizing pure CdIF-1, A Cadmium version of ZIF-8. It shows thermal stability, high porosity and structural similarity to ZIF-8. Different synthesis parameters, e.g. ratios of chemicals, temperature, reaction time, solvent, were tuned to get pure CdIF-1 crystals with improved morphologies. FTIR and single crystals analysis showed that comparing to ZIF-8, CdIF-1 has a less stiff metal to nitrogen bond and a larger framework. TGA was utilized for comparing the thermal stability between them.

50) PIL-DERIVED CARBON

PRESENTER: Rui Sun, Kelly M. Meek and Yossef A. Elabd

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

The development of new carbon-based materials with exquisite control over surface chemistry, carbon structure and form, surface area, pore size, and conductivity is of significant interest for numerous applications, including energy storage (e.g., capacitors). Recently, a few studies have demonstrated the ability to produce carbon from ionic liquids (ILs) and polymerized ionic liquids (PILs), both of which have unique physiochemical properties and result in carbon with various surface chemistries depending on the chemistry of the IL or PIL. However, to date, few studies have explored the relationship between the possible diverse PIL chemistries and the resulting PIL-derived carbon properties. In this study, PILs with various backbone/cation pairings (backbones: ethyl methacrylate, styrene; covalently attached cations: butylimidazolium, trimethylammonium, butylpyrrolidinium,) were successfully synthesized as carbon precursors. PIL-derived carbons with metallic luster were produced from this set of PILs via pyrolysis at 10 °C/min. Higher graphitization extent was obtained by PIL-derived carbons. Significant structure differences were observed between PAN-derived carbon (powder) and PIL-derived carbons (sheet). Cation has a considerable impact on graphitization extent and surface chemistry of the resulting carbon materials, while polymer backbone plays an important role in carbon yield and morphology. The design of PIL chemistry based on cation and

polymer backbone effects may be an approach to further optimize the characteristics of new PIL-derived graphitic carbon material for its subsequent implications in energy storage applications.

51) POROUS NANOMATERIALS WITH HIGH PERFORMANCE ENERGY STORAGE

PRESENTER: Dr. Wanmei Sun and Dr. Micah Green

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

porous nanomaterials are promising in applications, such as gas storage, catalysis, and energy storage. With satisfactory rate capability and cyclic stability, supercapacitor can boost or replace batteries to store energy as an electrical charge. Highly porous and well conducting electrodes are of special interesting. The working mechanisms of supercapacitors are intercalation, redox reactions or electrostatic adsorption on the active materials. Here we utilize two representative types of porous nanomaterials, carbon and tungsten trioxide (as a typical perovskite- like atomic configuration) with "external" high surface area and "internal" high surface area, respectively, to achieve high performance energy storage. Porous carbon is derived directly from kelp in ammonia at 700 °C, with enriched oxygen and nitrogen containing functional groups. The specific surface area of porous carbon is over 1000 m2/g with three-dimensional structure. This unique structure allows short ionic diffusion path, resulting in high volumetric capacitance (over 360 F/cm3), excellent energy density (~23.6 mWh/L), and outstanding cyclic stability. Different from "external" surface area, tungsten trioxide with intracrystalline tunnels shows high "internal" surface area from the atomic arrangement. The water molecular-sized porosity (~3.67 Å) in tungsten trioxide boosts the microporous adsorption, leading to higher specific capacitance and better cyclic stability. These two representative nanomaterials offer alternative approach to design, synthesize, and processing porous materials for related applications, including energy storage.

52) A LEADING INDICATORS-BASED DECISION SUPPORT TOOL TO PREDICT BLOWOUT EVENTS

PRESENTER: Nafiz Tamim[1], Delphine Laboureur[1], M. Sam Mannan[1] and A. Rashid Hasan[2]

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[2] *Harold Vance Department of Petroleum Engineering, Texas A&M University, College Station, Texas 77843*
TYPE OF PRESENTATION: POSTER

ABSTRACT:

Predicting a potential blowout scenario timely and efficiently is often a challenging task due to the complexities of drilling or other well intervention activities. Blowouts are usually preceded by kicks and early prediction of kick events can provide some precious time window to take control of the well in concern. A leading risk indicators-based approach for predicting gas kick or blowout events has been introduced in this work. A causal factors-based step-by-step approach for identifying comprehensive sets of leading indicators is presented. Leading indicators are divided into two broad sections – real-time indicators and long-term organizational safety performance indicators. With the real-time indicators, different decision support algorithms have been developed for better understanding of kick scenarios. A real-time indicator may not always successfully lead to a well control event, but the situation needs to be assessed carefully considering other factors and indicators. Such uncertainties are taken into account while developing these algorithms. For evaluating the relative importance of different leading indicators Bayesian Network models are developed. The key causal factors for well control barriers failure are identified by conducting fault tree analysis and appropriate indicators are linked with relevant causal factors in a Bayesian model. At the end, a list of effective leading risk indicators are presented for predicting primary well control barrier failure.

53) NATURAL GAS TO LIQUID TRANSPORTATION FUELS UTILIZING CHEMICAL LOOPING TECHNOLOGIES FOR SYNGAS GENERATION: PROCESS SYNTHESIS AND GLOBAL OPTIMIZATION

PRESENTER: William W. Tso[1,2], Alexander M. Niziolek[3,1,2], Onur Onel[3,1,2] and Christodoulos A. Floudas[1,2]

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[3]*Department of Chemical & Biological Engineering, Princeton University, Princeton, NJ*

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Even with advances in electric vehicles and improved vehicle fuel economy, the demand for liquid fuels in the transportation sector is projected by the U.S. EIA to remain steady through 2040. Liquid fuels produced from domestic feedstocks like natural gas could partially offset this demand and reduce dependence on foreign crude imports, enhancing national energy security and independence. Natural gas to liquid fuels (GTL) processes may also be economically promising due to an abundance of inexpensive natural gas in the United States.

In earlier works, the primary natural gas conversion technologies examined were syngas generation via autothermal reforming or stream reforming before further upgrading to liquid fuels via methanol synthesis or Fischer-Tropsch processes. Since high pressure operation limits the per-pass conversion in the reformers, larger reactor capacities and recycle streams were needed to increase the overall conversion, impacting the process economics.

Recent developments in chemical looping as an alternative for syngas generation from natural gas have expanded the potential GTL capabilities. Chemical looping reactors can be operated at lower pressures and offer close to complete conversion of natural gas in a single pass. Highly concentrated syngas can be produced without using pure oxygen, eliminating the need for additional air separation and syngas conditioning units. This could significantly reduce costs associated with GTL processes and improve the overall process efficiency.

This work incorporates two chemical looping technologies into a GTL process superstructure as alternatives to reforming for syngas generation. All process technologies are rigorously modeled and form a large-scale nonconvex mixed-integer nonlinear model (MINLP). A deterministic global optimization branch-and-bound algorithm is used to solve the MINLP.

Several case studies are investigated to compare chemical looping technologies against the reforming routes. The effect of plant capacity and production ratios on the overall profit is analyzed. Major topological decisions on process technologies will be discussed. Economic and environmental trade-offs will also be presented.

54) SYSTEMATIC ANALYSIS AND OPTIMIZATION OF ENERGY-WATER NEXUS

PRESENTER: Spyridon D. Tsolas, M. Nazmul Karim and M. M. Faruque Hasan

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

The existence and importance of the energy-water nexus is well known. Processes that need water to produce energy, and water providers who need energy may coexist. From plants to regions to countries, these energy and water sources, which also act as water and energy sinks respectively, exchange energy and water flows and interact with each other. A systematic analysis and understanding of the complex interactions and trade-offs between the energy and water sources and sinks is critical. This work focuses in the interconnection and circulation of water and energy flows, which is the essence of the nexus. To do that, we propose and utilize an energy load versus water load diagram. A visualization of the energy and water processes is provided, and a better understanding of the energy/water flows and their destinations is achieved. Then, through different configurations of the energy and water sources, based on the conversion factors, an existing system can be examined if it is redundant. That way the total energy and water production can be minimized, while maintaining and providing the same flows to the energy and water grids and

satisfying the same societal demands for water and energy. The other approach, examines if an existing system can increase the flows that go to the grid, while the total production of energy and water remains the same. Finally, an optimization model is developed based on the same principle of the graphical method and the two methods are tested on a fictional case and a real data case for the state of Texas.

55) A SYSTEMATIC APPROACH TO ALARM DESIGN WITH APPLICATION TO TENNESSEE EASTMAN PROBLEM

PRESENTER: Joshiba Ariamuthu Venkidasalapathy, Costas Kravaris and M. Sam Mannan

Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

When a process plant faces an abnormal situation, the alarm management system that is meant to assist process operators, may hinder effective remedial measures by simultaneously displaying several alarms, making it nearly impossible for the operator to identify the critical variable that needs immediate attention. This condition is known as 'alarm flooding'. This study focuses on efficient alarm identification which is the first critical step in designing the alarm system of a process plant.

We formulate a systematic approach to alarm identification wherein a subset of measured variables is chosen for configuration in the alarm system. The approach may be outlined as (i) Identification of potential hazardous scenarios, (ii) Simulation of these scenarios in order to quantify process measurement response time, (iii) Formulation of a mixed integer linear programming problem (MILP) that is solved using MATLAB/ GAMS. The solution to this problem gives a set of process variables that minimizes the time taken for abnormality detection while taking into account all potential hazards. Additionally, this optimal set ensures that the number of alarms activated for any fault is not more than a threshold number.

The formulation is as follows,

Objective function : $\text{minimize}_X \{ \max_j \{Detection\ time\ of\ faults\}$

where,

$X=[x_i]$

x_i = 1 if the measured variable is configured to alarm system

0 if the variable is not configured to alarm

i= {1, 2, ……, n}, n is the total number of measured variables

j= {1, 2, ……, m}, m is the number of faults

Such that,

$1 \leq \{ \text{Number of Alarms} \} \leq \text{Threshold Number}$

For this particular study, CPLEX solver of GAMS has been used which is based on the branch and bound algorithm.

The proposed approach is then applied to a benchmark industrial plant control problem, the Tennessee Eastman Process Control Problem [1], a well-defined simulator of a chemical process plant which is extensively used in process control research. It consists of a reactor, separator, condenser, stripper and a recycle compressor. The exothermic reactions involved and its operation under pressurized conditions make it a safety-critical plant, and hence a potential application for the proposed algorithm.

A number of major hazards were identified for this plant including control valve 'stiction' and sensor faults. The abnormal scenarios were simulated using the closed loop simulator in MATLAB environment [2], [3].The

simulations were carried out, one scenario at a time. The optimal set of process variables identified are 'Separator Pressure' and 'Purge gas composition- G component' for a threshold number of 2. The effectiveness of the approach depends on the simulator's predictive capability and thoroughness of Hazard Identification (HAZID) study.

56) IN-SITU MECHANISTIC INVESTIGATION OF AN ORGANIC RADICAL POLYMER CATHODE ON INTERFACIAL CHARGE AND MASS TRANSFER

PRESENTER: Shaoyang Wang, Fei Li and Jodie Lutkenhaus

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Organic radical batteries (ORBs), in which the organic radical polymer is used as the cathode and/or anode, have been considered as a promising alternative to conventional lithium-ion batteries, as the organic cathodes allow rapid charge transport and high cycling stability. One commonly studied stable nitroxide radical polymer, poly(2,2,6,6-tetramethylpiperidinyloxy methacrylate) (PTMA), is capable of a two-electron transfer process between its n-doped and p-doped states. The reported specific capacity of PTMA cathodes is between 77 to 220 mAh/g, depending on the charge/discharge conditions. Most previous research on PTMA is aimed at improving the electrode capacity and cyclability either by adding highly conductive materials or by optimizing the radical polymer synthesis. However, the charge storage process and the electrode/electrolyte interface in such systems are not understood on the molecular level. Here, we present the first application of in situ electrochemical quartz crystal microbalance with dissipation monitoring (EQCM-D) towards understanding the charge storage process in PTMA cathodes. EQCM-D monitors changes in frequency and dissipation of a PTMA-coated quartz crystal during controlled electrochemical interrogation (cyclic voltammetry and chronoamperometry). The change of mass and shear viscosity can be further obtained from viscoelastic modeling of the raw data, leading to a quantitative view of mass transport associated with the doping process. The heterogeneous electron-transfer rate constant and diffusion coefficient are estimated from the electrochemistry data. Here, we specifically investigate the effect of different lithium electrolyte salts on the charge transfer process. Each salt gives different charge storage behavior and mass transport, which may be attributed to varied polymer-dopant and dopant-solvent interactions.

57) AEROSOL GENERATION APPROACH AND COMBUSTION SIMULATION

PRESENTER: Shuai Yuan, and M. Sam Mannan

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

The flash points of heat transfer fluids used in heat exchangers are normally higher than 200℃, which makes people ignore their fire and explosion potential. In an incident in Milliken Carpet factory on 31 January 1995 that resulted in over $400 million total loss, the cause of this incident was attributed to the leak of heat transfer fluid in the form of aerosol at high pressure. An ignition source ignited the heat transfer fluid aerosol when the surrounding temperature is below its flash point. Although Eichhorn introduced the concept of aerosol flammability limits, the values of aerosol flammability limits are still unclear. Understanding the aerosol formation mechanism and aerosol flammability region helps process designers to implement inherently safer design to minimize the risk.

Electrospray method is used to generate aerosol. The liquid fluid with sufficient electric conductivity is dispensed by syringe pump through the small nozzles. The nozzles are aligned in a few kilovolts electric field. Under the influence of electric field force, the fluid is atomized to small droplets. The advantages of electrospray method compared with other methods are the droplet size controllability and spray stability. Various literature has shown that the liquid properties, such as liquid conductivity, surface tension, permittivity and viscosity, play the most important roles in determining droplet size. In the heat transfer fluid chosen to study the aerosol, the droplet size is controlled by

changing the conductivity of fluid by adding additives, adjusting the electric field intensity and shifting the fluid feeding flow rate.

An open source CFD software, OpenFOAM, is applied to simulation the generation and combustion process of aerosol droplets. The target of this study is to compare the simulation results with the experiment result in order to validate that the user defined solver has the ability to simulate these two process, generation and flame moving upward.

58) HIGH-FLUX HYBRID MEMBRANES FOR EFFECTIVE OIL-WATER SEPARATION FROM OIL-CONTAMINATED WATER

PRESENTER: Glenn Zeng[1], Lecheng Zhang,[1,2] Dali Huang[3] and Zhengdong Cheng*[1,2,3]

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Recent oil spills and the rapid expansion of petrochemical industries have highlighted the challenge of effective oil-water separation. Developing a filtration platform based on new surface modification strategies that exhibit good oil-water separation, particularly in a complex environment, is highly desirable for purposes of environmental clean-up. Herein, we present a polymer-modified filter paper (PMFP) with an underwater superoleophobic surface fabricated via a facile dip-coating process. The as-prepared polymer-modified filter paper not only separates the oil-water mixture in gentle environment, but perform effectively in harsh environments, including high salt concentrations, extreme pH, and oil-in-water emulsions with surfactants, suggesting its great potential for large-scale industrial applications.

59) THE EFFECT OF WATER ON THE THERMAL TRANSITION OBSERVED IN POLY(ALLYLAMINE HYDROCHLORIDE)-POLY(ACRYLIC ACID) COMPLEXES

PRESENTER: Yanpu Zhang, Ran Zhang, Maria Sammalkorpi and Jodie L. Lutkenhaus

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Polyelectrolyte complexes (PECs) are receiving increasing attention because of their stimuli-responsive behaviors with ionic strength, pH, and temperature. Of these, temperature is particularly intriguing in that PECs undergo a glass-melt transition whose origin remains debatable. Here, we present the thermal behavior of PECs containing weak polyelectrolytes poly(allylamine hydrochloride) (PAH) and poly(acrylic acid) (PAA) as influenced by water content and complexation pH. These are investigated using modulated differential scanning calorimetry (MDSC) and dynamic molecular simulation. MDSC revealed a glass-transition-like thermal transition (Ttr) that decreases with increasing hydration and with decreasing complexation pH. It is shown that water has a plasticizing effect by molecular simulations and comparison with the Fox equation. Simulations show an increasing number of water-polymer hydrogen bonds within the hydrated complexes as water content increases. Complexation pH influences the thermal transitions by tuning the polymer charge density and then the structure and composition of the PEC. These results support the hypothesis that the transition is caused by a restructuring of the water hydrogen-bonding network within the PEC that then allows for subsequent chain relaxation.

60) ADVANCED HEAVY GAS DISPERSION MODEL WITH LESS TIME AND HIGHER NEAR-FIELD ACCURACY THAN CFD-BASED SIMULATION

PRESENTER: Jiayong Zhu, Delphine Laboureur, and M. Sam Mannan

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX-77843

TYPE OF PRESENTATION: POSTER

ABSTRACT:

Many substances released from industries are toxic, flammable, or even both. When these substances are accidently released to the atmosphere, potential harm could threaten human health and environment. Hazardous materials, such as chlorine and hydrogen sulfide, are heavy gases, which have larger density than air. Heavy gases tend to move toward the ground where wind speed decreases and gas cloud dilution processes reduces. Thus, heavy gas maximizes the dangerous effects.

Effective heavy gas dispersion models are crucial to provide decision makers quick assessment on potential impacts. Based on results from Computational Fluid Dynamic (CFD) models simulation and experiment data, this paper proposes an advanced model accounting for wind speed, obstacles, and turbulence effects. Unlike CFD models, which takes large amount of time to set up, mesh, calculate and post-analysis, the proposed model is able to give a quick analysis on concentration distribution. Additionally, since turbulence models in CFD models are averaging the eddy effects, near-field estimations are often under-estimated. The proposed model overcomes this disadvantages.

61) ENHANCING PHOTOCATALYTIC CO2 REDUCTION BY COATING AN ULTRATHIN AL2O3 LAYER ON OXYGEN DEFICIENT TIO2 NANORODS THROUGH ATOMIC LAYER DEPOSITION

PRESENTER: Huilei Zhao and Ying Li

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TYPE OF PRESENTATION: POSTER

ABSTRACT:

Anatase nanorods (ANR) of TiO2 with active facet {100} as the dominating facet were synthesized and oxygen deficient TiO2-X nanorods (ReANR) was prepared by reducing TiO2 using NaBH4. On the surface of ReANR, a thin layer of Al2O3 was coated by atomic layer deposition (ALD), and the thickness of Al2O3 was tailored by varying the cycle number (1, 2, 5, 10, 50, 100, or 200) of ALD operation. The growth rate of Al2O3 was 0.25 Å per cycle as evidenced by high-resolution transmission electron microscopy, and the amorphous structure of Al2O3 was determined based on X-ray diffraction results. ANR, ReANR and Al2O3 coated ReANR were tested for CO2 photoreduction with water, with CO and CH4 as the major and minor products, respectively. Compared with ANR, ReANR had more than 50% higher CO production and more than ten times higher CH4 production due to the oxygen vacancies that possibly promoted CO2 adsorption and activation. With less than 5 cycles of ALD, Al2O3 coated ReANR had enhanced overall production of CO and CH4 than uncoated ReANR, with 2 cycles being the optimum, about 40% higher overall production than ReANR. Whereas, when more than 5 cycles were applied, both CO and CH4 production decreased with increasing number of ALD cycles. Photoluminescence (PL) analysis showed the both 2 cycles and 200 cycles of Al2O3 ALD coating layer on the ReANR were able to reduce the charge carrier recombination rate, likely because of the passivation of surface states. However, a relatively thick layer of Al2O3 may act as an insulation layer to prohibit electron migration to the catalyst surface. This work gives valuable insights on the application of ALD coating on photocatalysts to promote CO2 photoreduction to fuels.