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CHEMICAL ENGINEERING GRADUATE STUDENT ASSOCIATION

6th ANNUAL RESEARCH SYMPOSIUM

ABSTRACT BOOK

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(1) Li Dendrite Nucleation from First Principles Perspective

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Given the demands of modern society, current chemical energy storage needs significant improvement. Advanced battery technology research has focused on the use of Lithium metal anodes to increase performance for Li-ion, Li-sulfur and Li- air batteries. Unfortunately, the use of these anodes causes several problems for battery operation such as the formation of dendrites. In the cycling of lithium anodes, the lithium will be deposited in a way that lithium metal tendrils or spikes grow on the surface of the electrode. These dendrites can cause the short circuiting and other mechanical problems that hurt performance and can even lead to significant safety concerns. Researchers have been focusing counteracting dendrite growth and formation from an experimental and practical approach but there has been a lack in fundamental understanding of how lithium dendrites form and grow. We used first principles simulations to study the nucleation, growth and properties of lithium clusters to determine the basic principles that govern dendrites. By exploring the reduction chemistry with small clusters, general principles can be derived that will help intelligently guide experimental and other modeling research to better battery design. We found that the reduction of Li ions is highly favorable regardless of position on the nucleating cluster which indicates that other factors are more important to the direction of cluster growth like the electrostatic potential that corresponds to a given electronic density distribution. With this information, the evolution of lithium clusters was investigated to connect clusters to dendrites as well as the influence of a copper substrate and SEI species. These models provide a methodology that gives a base for further study of dendrite fundamentals that can be easily extended to engineer high performance battery technology.

Keywords: battery, modeling, lithium-sulfur

(2) Radio frequency processing of preceramic polymer nanocomposites and its application

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In this work, we have demonstrated an oven-free and mold-free heating route to convert preceramic polymers to silicon carbide with carbon nanomaterials as RF susceptors. Silicon carbide is prized for its high thermal stability and low density and can be produced by slow conventional oven heating of polycarbosilanes. We show that addition of multiwalled carbon nanotubes to polycarbosilanes results in rapid and volumetric heating upon exposure to radio frequency fields and microwaves. Thermogravimetric data shows that the extent of cure for RF cured samples is around 95 %. We have also studied microwave heating of polycarbosilanes-MWCNT composites and the resulting crystal structure. We demonstrate this method for 3D printing of silicon carbides by a successive deposition and RF curing approach. We have also shown that this method can be used to cure polycarbosilanes to make SiC fibers with shape retention.

Keywords: ceramics, 3D printing, polymers

(3) Room Temperature Solid-State Lithium Polymer Battery with Polyionic Liquid Pentablock Terpolymer Electrolyte

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Lithium ion batteries are currently the leading commercial technology for portable electronic devices and electric vehicles. However, new solid polymer electrolytes (SPEs) that comprehensively possess the preferred properties of high ion conductivity, high electrochemical stability, robust mechanical properties, and good film forming properties, are required to improve the safety and lifetime of lithium ion batteries. Although diblock copolymers have been explored as SPEs and can potentially provide the orthogonal properties of high ion conduction and high mechanical strength simultaneously in a solid-state material, there are limitations to diblock copolymer-salt mixture systems, such as a limited set of morphologies, and a lack of means to achieve simultaneous combination of more than two properties (e.g., conductivity, strength, flexibility). Compared to diblock copolymers, multiblock polymers involve more than two polymer chemistries and therefore enable the possibility to conjoin many of the desired properties, such as high ion conductivity, mechanical strength, flexibility, good film forming properties, and high electrochemical stability all into a single materials platform. In this study, a lithium ion conducting polyionic liquid pentablock terpolymer (PILPTP) was investigated as a solid polymer electrolyte (SPE) for lithium ion batteries. The morphology, chemical, thermal, mechanical, and electrochemical properties were examined as function of ionic liquid composition, cation chemistry, and film processing conditions. Coin cell Li4Ti5O12/SPE/LiCoO2 batteries were fabricated with the lithium ion conducting PILPTP as the SPE and room temperature battery performance was demonstrated at high capacity and high cycle life. Overall, this work suggests, for the first time, that lithium conducting polyionic liquid multiblock polymers can be promising electrolyte candidates for developing safe and high performing room temperature solid-state lithium ion batteries.

Keywords: multiblock polymer, battery, ionic liquid

(4) Flagellar hydrodynamics in Bacillus subtilis

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For bacteria, the rotation of flagellar motors generates a thrust on the cell body and the magnitude of thrust determines the swimming speed. Swimming of monotrichous cells can be modeled as a single sphere coupled to a helical filament, and hydrodynamic theories model the system fairly well. However, in peritrichous cells, the thrust varies not only as a function of flagellar polymorphic form and arc lengths, but also the flagellar numbers. The linear swimming speed is governed by a combination of these parameters, as well as cell geometry and hook/filament flexibility. In addition, the torque developed by flagellar motors is dependent on the hydrodynamic drag on the filaments, which is influenced by filament-filament hydrodynamic interactions. Here, we experimentally test hydrodynamic theories that predict an independence of swimming speed, and hence flagellar thrust, on the number of filaments. Using particle tracking algorithm and fluorescent-labeling techniques, the swimming speeds of B. subtilis and E. coli were shown to be similar despite the fact that the former carried almost twice the number of filaments as the latter. This is consistent with the predicted independence of swimming speed on filament numbers. Surprisingly, B. subtilis cells were longer and the motor torque was considerably lower, which precludes higher speeds. Preliminary data suggests the need for a revision of theories to model peritrichous motility accurately.

Keywords: Hydrodynamics, Bacterial Motility, Biophysics

(5) Novel technique to target bacteria, Pseudomonas aeruginosa, via hetero-multivalent binding

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Pseudomonas aeruginosa (PA) is among the three most critical pathogens which are in the need of new antibiotics. Unlike the classic lock-and-key-binding model, we discovered that lectins on such bacteria often exhibit hetero-multivalency in which multiple binding domains in a single lectin bind with different kinds of ligands concurrently. Inspired by this nature of bacterial adhesion to host cells, we developed an innovative targeted drug delivery system to enhance drug retention at the infection site. Liposomal drug carriers were chosen because liposomes provide critical two-dimensional glycolipid mobility to enhance multivalent interactions. Because of the reduced dimension of ligand diffusion, the reaction rates of the subsequent bindings are at least 104 times higher than the first binding event. This rate-enhancement mechanism, Reduction of Dimensionality (RD), dramatically increases the efficiency of multivalent binding, such that upon completion of first attachment, even low-affinity ligands can contribute to liposome attachment to bacteria. Traditionally, targeted drug delivery schemes have decorated drug carriers with high-affinity ligands only. The RD mechanism suggests that we can simultaneously utilize both high- and low-affinity ligands to achieve higher binding avidity and specificity. To demonstrate this concept, we exploited the ability of PA to adhere to eukaryotic cells. We successfully found a new PA-specific ligand, lactosylceramide (LacCer), from eukaryotic cells, and improved the liposome retention rate up to 400% by blending LacCer with the other known PA-specific ligand, Gb3, in vitro. In addition, we demonstrated that these liposomes decorated with glycolipids could penetrate through physiological barriers and reach the infection sites in a thigh infection mouse model. Our in vitro and in vivo studies indicated this unique bio-mimetic approach not only improves the targeting efficiency towards PA, but also reduces the off-target binding.

Keywords: Targeted drug delivery, Hetero-multivalent binding, bacteria

(6) Dynamic Power Plant Scheduling with Flexible Carbon Capture in Uncertain Electricity Markets

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While power plants produce electricity from fossil fuels, they are responsible for more than 30% of the global anthropogenic carbon dioxide emissions. One way to reduce emissions is to capture carbon dioxide from the power plant flue gas through solvent-based absorption. However, high energy requirement in solvent regeneration limits widespread deployment of the technology. To overcome this limitation, we consider flexible power plant operation with an integrated carbon capture unit which varies its load in response to fluctuating electricity prices. A deterministic model with perfect foreknowledge of electricity prices is extended to a stochastic model to incorporate price uncertainty. A multi-stage stochastic programming approach is applied to determine an optimal power production and carbon capture schedule for maximizing daily operating profit. Low-complexity surrogate models are developed for optimal action policy at each hour, which reduce the computational complexity in an optimization framework. The results represent the optimal hourly action policy as continuous functions which would enable the power plant operator to take decisions under uncertain prices. These models are then used to calculate total optimal profit for different possible scenarios of electricity price. Through this framework of flexible operation, power plants can sustain 20% more profit while achieving up to 90% reduction in emissions.

Keywords: Multi-stage optimization, Stochastic dynamic programming, Clean energy

(7) Toward Supply Chain Optimization of Renewable Energy Carriers

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A main challenge of renewable energies such as solar and wind is their intermittency. Wind and solar availabilities fluctuate daily, seasonally, and geographically. Moreover, they are often temporally and spatially asynchronous with our energy demands. One proposed solution to the intermittency problem is to store energy during periods and in areas of excess supply and to utilize the stored energy during periods and in areas of excess demand. An option for energy storage is using chemicals such as hydrogen1, ammonia2, or methanol3. Unlike batteries, chemicals are more energy dense, easily transportable to the end-user, and offer flexibility in terms of end-usage. They act as energy carriers, moving solar and wind energy from one location to another.

While the industrial production of these chemicals is well-established, the integration of renewable energies into the manufacturing process and supply chain is an unresolved task. Toward this latter aim, in this work, we describe the development of a supply chain model framework to systematically analyze the potential of solar and wind to displace energy demand through the deployment of energy carriers. The framework investigates the various tradeoffs and competing options for building an energy carrier infrastructure, and through optimization, the best energy carrier network is elucidated. We will highlight the results on a Texas case study and showcase the feasibility of energy carriers.

Keywords: renewable energy, energy carriers, optimization

(8) Reliability Analysis in Synthesis of Direct Water Recycle Networks

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The development of Eco-Industrial Parks (EIPs) has drawn much attention due to the growing concern in sustainability. The main idea of an EIP is to form an interdependent production infrastructure that combines chemical plants for integrations of materials, energy, water, utility system, and waste management. However, such highly integrated processes usually result in complex systems with a large number of connections for mass and heat integration. Thus, a minor incident of one individual plant could lead to a potential decrease in the overall production rate or even complete shutdown of the entire production site. The economic loss due to the event could outweigh the benefits of an integrated system. Reliability analysis should always be included for both design and operation phases. In this work, a systematic approach is proposed to quantify unit and system reliability. An optimization framework is then developed to integrate reliability factor into the current model for direct water recycle networks, which includes methods to improve the overall system reliability. The epsilon-constrained method is used to solve the multi-objective optimization problem. The result illustrates Pareto optimal solutions that demonstrate the trade-off between network cost and reliability. It could help guide the decision-making process for choosing the optimal design and operating strategy for the water recycling system to ensure a reliable EIP.

Keywords: Process Integration, Reliability, Eco-Industrial Parks

(9) Dynamically-Intensified Adsorption-Reaction Processes for Unconventional Natural Gas Utilization

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Unconventional and distributed feedstocks such as shale gas, landfill gas and associated natural gas are predicted to meet majority of future energy demands. For utilizing these unconventional resources in stranded locations, sorption enhanced reaction processes (SERP) with intensified reaction-separation phenomena can be effectively deployed for reaction, conversion and storage purposes. In SERP systems, in-situ reaction byproduct removal from the reaction gas mixture, by a solid adsorbent, enhances production of the desired product. The advantages of SERP technology include compactness, energy efficiency, lower capital intensity, higher reaction conversions, and enhanced product quality. For synthesis and optimization of periodic SERP systems for unconventional gas utilization, we develop a generalized reaction-adsorption modeling, simulation and optimization (GRAMS) framework.

GRAMS is based on a nonlinear algebraic and partial differential equation (NAPDE)-based model which simultaneously identifies optimal SERP cycle configurations, design specifications and operating conditions. The major modeling contributions include a generalized boundary-condition formulation and a unified representation for optimal selection of discrete operation modes and flow directions using continuous pressure variables. An in-house simulation-based constrained grey-box optimization algorithm is incorporated in GRAMS to obtain optimal (i) SERP cycles, (ii) process design parameters and (iii) operating conditions. The framework has been used for designing three SERP systems, namely sorption-enhanced steam methane reforming (SE-SMR), sorption-enhanced water gas shift reaction (SE-WGSR) and sorption-enhanced methanol synthesis (SE-MeOH).

Keywords: Process Design, Process Intensification, Process Optimization

(10) Modeling and control of proppant distribution of multi-stage hydraulic fracturing in horizontal wells

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In shale rock formations, multiple hydraulic fracturing treatments with slick water are generally used to stimulate the recovery of natural gas and oil. The slick water can create massive hydraulic fractures, but it is inefficient at suspending proppant due to the low-viscosity, resulting in the creation of significant proppant bed at the bottom of the fracture, which will influence the subsequent proppant transport mechanism inside fracture. Currently available hydraulic fracture simulators mainly focused on simultaneously propagating multiple fractures considering stress shadow effects without considering this proppant transport phenomena. As of now, the simulation of proppant transport has mainly focused on simple fracture geometry, i.e. a single, planar fracture. Even though some efforts have been made to simulate the proppant transport using the Eulerian-Eulerian method, dense proppant transport and proppant bed formation were not considered. Recently, the Eulerian-Lagrangian method was used to model particle movement, which is highly computationally expensive to be incorporated into simultaneously propagating multiple fractures model. Motivated by these considerations, the proposed research will first address the development of a new high-fidelity model by explicitly accounting for stress shadow effects as well as proppant transport.

The hydrocarbon production through these multiple fracture networks is strongly dependent on the proppant distribution within the fractures. Therefore, the proppant distribution at the end of pumping in simultaneously propagating multiple fractures must be regulated by developing model-based pumping schedules. In this work, utilizing the new high-fidelity model, we will focus on introducing a new model-based control algorithm to compute online pumping schedules that compensate for stress shadow effects, which will be able to generate uniform proppant distribution in simultaneously propagating multiple fractures.

Keywords: Optimal pumping schedule, Hydraulic Fracturing, Model predictive control

(11) A Multiparametric Programming Based Approach to Integrate Design, Scheduling, and Control of a Batch Process

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Integrating short term (control), middle term (schedule), and long term (design) decisions has been shown to improve the operability and profitability of batch processes. The interactions between these distinct time-scale decisions allow for opportunities to (i) replace fixed recipe-based schedules with detailed model-based schedules, (ii) build design dependent schedule aware controllers, and (iii) reduce capital costs by circumventing overdesigned processing units. While the efficiency of simultaneous decision making in process systems is greatly acknowledged, the methodology/procedure to achieve an effective integration is still an open question due to the order of magnitude differences in the time scales of the constituent problems, as well as their respective objectives. The most recent advances within the last decade depict a promising basis for further improvement.

In this work, we present a unified framework to simultaneously determine the optimal codependent short term and middle term operating strategies of a batch process for a range of market conditions, while minimizing the capital costs. A single high fidelity model is utilized to develop (i) multiparametric rolling horizon optimization (mpRHO) strategies as a function of process states and time variant market conditions, and (ii) multiparametric Model Predictive Control (mpMPC) for effective set-point tracking. The design of the process is accounted for as an additional unknown bounded parameter in the offline operational strategies. The offline nature of mpRHO and mpMPC strategies allows for integration in the design optimization of the process, i.e. minimizing the capital costs. The framework is showcased on a single non-isothermal batch reactor.

Keywords: enterprise-wide optimization, multiparametric programming, process scheduling

(12) Data-Driven Optimization with Implicit Constraints: Application to an Ethane Steam Cracking Process

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Data-driven modeling relies on different sampling strategies that provides an initial plan for the controlled experiments on problem simulators, which is commonly known as the Design of Experiments (DoE). The DoE provides possible candidate locations for input variables within the pre-defined box-constraints in such a way that these experiments capture a variety of system dynamics. However, this statistical procedure is not guided by the physical information that entails an engineering process. Thus, a subset of candidate points may result in unphysical and/or undesirable outcomes, such as an early termination of the problem simulator due solving a numerically unstable problem (stiff Ordinary Differential Equations, ODEs). This implies that a constraint between the optimization variables exists, in which the explicit analytical formulation of this is unknown. The aim of this work is to handle implicit constraints that exists between the input variables and guide the initial sampling strategy in such a way that the numerically unstable combinations of input variables are filtered out, leaving only an appropriate set of samples for simulating the problem. This problem is formulated as nonlinear classification problem using Support Vector Machines (SVM) where an optimal hyperplane, separating numerically stable and unstable samples, is built to implement an implicit constraint for the input space. The model is trained and cross-validated using a large set of simulated samples offline, and then incorporated in the ARGONAUT framework to assess the feasibility of the candidate points a priori to sample collection. This methodology has been tested on an ethane steam cracking process, where the continuity, energy and momentum balances are characterized by stiff ODEs. The results show that SVM model provides a highly accurate implicit constraint and helps the grey-box optimizer to return feasible profitable solutions to the steam cracking optimization process.

Keywords: Data Analytics, Optimization, Ethylene Production

(13) Data-driven identification of interpretable reduced-order models using sparse regression

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Reduced-order models (ROMs) can be thought of as computationally inexpensive mathematical representations, of a high-fidelity dynamical model that preserves essential behaviors and dominant effects that offer the potential for near real-time analysis. Developing physically interpretable reduced-order models is critical as they provide an under- standing of the underlying phenomena apart from computational tractability for many chemical processes. In this work, we approach the reduced order modeling problem of nonlinear dynamical systems from the perspective of compressive sampling and sparse regression. We rely solely on time series data collected at a fixed number of spatial locations to identify parsimonious and physically interpretable ROMs. The fundamental assumption in this method is that there are only a few relevant terms that dictate the system dynamics. This is a reasonable assumption which holds for many physical systems as long as a set of appropriate basis functions is selected. Within this context, we perform nonlinear sparse regression on a large library of potential candidate functions to determine the fewest terms that most accurately represent the data. Therefore, the resulting ROMs are functions of the original system states and inputs, and the identified dynamical system is interpretable. The method balances model complexity and accuracy by selecting a sparse model that avoids overfitting to accurately represent the system dynamics when subjected to a different input profile. By applying to a hydraulic fracturing process, we demonstrate the ability of the developed models to reveal important physical phenomena such as proppant transport and fracture propagation inside a fracture. It also highlights how a priori knowledge can be incorporated easily into the algorithm and results in accurate ROMs that are used for controller synthesis.

Keywords: Reduced-order model, Sparse regression, Hydraulic fracturing

(14) Building block-based design and intensification of chemical processes

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Process intensification provides means for more sustainable, cost effective, smaller and safer designs compared to their conventional counterparts. Often times, intensification is realized through capturing the synergy between different process phenomena. Identification of such intensification opportunities can be facilitated through a departure from unit-operation-based design paradigm which has been the modus operandi since the last century. Accordingly, several process intensification methods have been developed in the past that rely on process phenomena, mass/heat exchange modules and/or tasks. However, it remains a challenge to systematically identify the optimal intensified flowsheets for a given design problem. To this end, building block-based approach [1] provides unique advantages for systematic process design and intensification. In this work, we will show that this representation approach leads to an optimization-based systematic method for process intensification. Unlike the traditional superstructure-based approaches, our representation is formed by building blocks positioned on a two-dimensional grid and relies on physicochemical phenomena to automatically generate optimal intensified flowsheets. By using either single or multiple building blocks, many physicochemical phenomena can be represented. This results in a mixed-integer nonlinear optimization (MINLP)-based model that describes the superstructure. We will demonstrate the benefits of the building block-based design approach in terms of systematic process intensification through several case studies with a special focus on natural gas utilization systems, energy-intensive separations, and reactive separation processes.

[1] Demirel, S. E., Li, J., and Hasan, M. M. F., 2017. Systematic Process Intensification using Building Blocks, Computers and Chemical Engineering, 105, 2-38.

Keywords: Process Intensification, Process Optimization, Sustainable Production

(15) Enlarging the domain of attraction of Local Dynamic Mode Decomposition with control technique: Application to hydraulic fracturing

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Local Dynamic Mode Decomposition with control (LDMDc) technique combines the concept of unsupervised learning and DMDc technique to extract the relevant local dynamics associated with highly nonlinear processes to build temporally local reduced-order models (ROMs). But the limited domain of attraction (DOA) of LDMDc hinders its widespread use in prediction. To systematically enlarge the DOA of the LDMDc technique, we utilize both the states of the system and the applied inputs from the data generated using multiple 'training' inputs. We implement a clustering strategy to divide the data into clusters, use DMDc to build multiple local ROMs, and implement the k-nearest neighbors technique to make a selection amongst the set of ROMs during prediction. The proposed algorithm is applied to hydraulic fracturing to demonstrate the enlarged DOA of the LDMDc technique.

Keywords: Reduced-order modeling, Dynamic mode decomposition, Hydraulic fracturing

(16) Simultaneous Design and Control of an Inherently Safer Extractive Distillation Column

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Current inherently safer design strategies in the early stages of design focus on reducing the overall hazard of a process without considering its operability. The process is first designed to be inherently safer with respect to a nominal, steady state case and then, after the process is designed, layers of protection are added and operability issues are addressed. However, the process design heavily impacts the final process' overall operability. In the early stages of design, it is necessary to consider of both the inherent hazard contained within the process and the ease by which these hazards can be controlled. With the dynamic behavior of process systems becoming increasingly complex, the consideration of operability issues in the design stage becomes even more necessary to prevent incidents. Hence, a considerable amount of research has been done to simultaneously optimize the design and control system of distillation columns, but no such approach has integrated inherent safety, only seeking to produce an economically optimal design rather than a safe one.

The objective of this research is to implement a strategy to simultaneously design and control an inherently safer distillation column. The PARametric Optimization and Control (PAROC) framework is used as a basis for the simultaneous design and control of a distillation column. The inherent safety index is incorporated into the PAROC framework, and the distillation column is simultaneously optimized for optimal control, design, and safety. The integration of inherently safer design and control substantially reduces operability issues that result from an uncontrollable process design and allow for greater tolerance and ease of control.

Keywords: Process Design and Development, Inherent Safety, Operability

(17) Effects of obstacle configuration on flame propagation regimes and explosion severity

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Flame propagation and explosion behavior of hydrogen mixtures remain critical issues for explosion safety in nuclear power plants and refineries. Although extensive efforts have been made to understand the underlying mechanisms affecting flame acceleration and explosion severity in obstructed enclosures, most of the studies address obstacles with uniform distribution. This uniformity is characterized by constant obstacle spacing, shape, and blockage ratio, and may not be representative of the layout in actual industrial facilities. Therefore, the objective of this work was to investigate the influence of unequal area blockage and obstacle spacing on the leading shock wave speed and overall overpressure during flame propagation. Experiments were performed in a closed pipe with 38-mm internal diameter and a total length-to-diameter ratio (L/D) equal to 73. Two ring-shaped obstacles with 5-mm thickness were used during each test. The arrangement between obstructions in the test vessel was changed in terms of blockage ratio (increasing, decreasing, and equivalent) and obstacle distance (1D, 2D, and 3D). Premixed hydrogen/oxygen mixtures at stoichiometric concentration were considered at three different initial pressures – 50, 100, and 150 torr. The aim was to identify layout parameters that increase the overall overpressure and reduce run-up distance when detonation-to-deflagration (DDT) takes place. From the conditions tested, the increasing blockage ratio has a more significant impact on the overall maximum pressure and the run-up distance.

Keywords: gas explosion, explosion safety, flame acceleration

(18) Experimental Study of Electrostatic Hazard inside Scrubber Column Using Response Surface Methodology

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Electrostatic ignition has triggered significant fire/explosion incidents in liquid processing industries including chemical, oil/gas, food, pharmaceutical and transportation. In this work, the impact of gas-velocity and temperature on the electrostatic energy accumulation in a scrubber column was studied. An in-situ charge measurement apparatus combined with a particle scattering laser function was installed inside a pilot-sale column filled with water through which nitrogen was sparged; the formed aerosol particle size distribution, concentration, mass and charge were measured simultaneously. Response surface methodology was employed to construct a quadratic model correlating the electrostatic energy response with the gas velocity and column temperature. Four scenarios were considered and their capacity to provoke ignition was evaluated. Temperature was found affect the charged aerosol droplet size but also to facilitate the charge relaxation in the liquid phase. The faster the gas velocity the higher the electrostatic energy accumulation and the probability of ignition. In the presence of non-grounded conductors, the maximum electrostatic energy from spark discharge was found above the minimum ignition energy of some flammable chemicals and poses as significant fires or explosion risk. In contrast, if there is no ungrounded conductor, the corona discharge was found not sufficient for electrostatic ignition in the range of temperature and gas velocity in this study. To reduce the electrostatic hazards, it is recommended to remove ungrounded conductors within the column. And the gas flow should be maintained at minimum if ungrounded conductors are present.

Keywords: Process safety, Aerosol hazards, Absorption column

(19) Safer design and operation of Proton Exchange Membrane Fuel Cells

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One of the most promising technologies for moving towards a hydrogen economy is the proton exchange membrane fuel cell (PEMFC) due to its low operating temperatures, low weight and volume, high power density and short startup time. This technology has begun to be used as in the form of fuel cell electric vehicles (FCEVs). However, a major hindrance towards making PEMFCs competitive with hydrocarbon-based combustion engines is the higher costs owing to lower durability of these systems. Specifically, the reliability of membrane exchange assembly (MEA) has been identified to be the key issue contributing towards overall lower durability of these systems. This decrease in reliability is attributed to membrane degradation leading to the overall PEFMC system degradation. Apart from contributing to decreased performance and higher cost, PEMFC degradation has been identified through fault tree analysis as one of the root causes that can lead to hydrogen leak and subsequent explosion.

The consequences resulting from hydrogen leak and explosion in a PEMFC system can be disastrous, especially from the perspective of vehicular application. Therefore, to mitigate the risk associated with explosion in PEMFC system and to achieve the required levels of performance, it is essential to study the degradation of PEMFC membrane in depth. This study deals with understanding the fundamentals of PEMFC degradation through modeling using computational fluid dynamics (CFD). More importantly, the degradation mechanism is quantitatively related to the probability of explosion of the PEMFC system using fault tree analysis. Therefore, an important inference from this study will be the design and operation alternatives for PEMFC that mitigate membrane degradation leading to improvement in both performance and safety of the system.

Keywords: Fuel cells, Performance, Explosion

(20) Homeomorphic Isomerism in Macrobicycles

Lars Erik Andreas Ehnbom[1], Michael B. Hall[1], John A. Gladysz[1]

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Macrobicyclic compounds have been proposed to interconvert from an in-in
(ii) form to an out-out (oo) form via a process named homeomorphic isomerism. This mechanism would require one of the three bridges to be threaded through the ring formed by the remainder of the structure, and proceed via a "cross-chain"
(cs) intermediate. Structural evidence for this mechanism is limited and our objective was to understand, if using simulated annealing to sample conformations of these macrobicyclic compounds, could lead to the observation of cs isomers. At which cage size is the homeomorphic process active? We further sought to gain insight of the relative thermodynamic stability of ii and oo as a function of cage size. Additional spectroscopic insight was sought, as this would further support the previous hypothesized spectroscopic assignments. A combination of calculation methods were used. Electronic structure methods (e.g. density functional theory) was used for spectroscopic analysis and to probe stability differences whereas molecular dynamics was used to sample the conformational space. We found that the homeomorphic isomerism can be supported but not for all cage sizes. cs are only observed when at least 13 methylene linkers are present. By expanding the size of the cage, the frequency of cs increased. With respect to the mechanism, cs structures of the type shown and an asynchronous process is supported. We conclude that pyramidal inversion does not participate in this process based on a frequently observed cs intermediate that is almost isoenergetic with the oo isomers. ii isomers are more stable than oo species by ca. 5 kcal/mol. These investigations will help design container molecules with appropriately sized macrobicycles which can have the homeomorphic mechanism turned on or off based on size.

Keywords: Homeomorphic Isomerism, Computational Insight, Macrobicycles

(21) Development of the optimization model for the shale gas prudction with water management considering the control of hydraulic fracturing system in the unconventional wells

Yuchan Ahn[1], Joseph Kwon[1], Prashanth Siddhamshetty[1], Kaiyu Cao[1]

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This study is presented to develop the optimization model for the production of the shale gas and determine the optimal design by integrating the control design of hydraulic fracturing system and the supply chain network for the operation of the shale gas production considering shale gas and water management. The objective of this model is to decide the profit of the shale gas production system by using the several values, such as freshwater demand and production amount of the shale gas determined by the control design of the hydraulic fracturing system, in the supply chain network model. The control design of the hydraulic fracturing system, which can regulate the uniformity of proppant bank heights along the fracture at the end of pumping, determines (1) optimal length and width of the fracture, and optimal number of fractures, and (2) freshwater demand, flowback water generation, and production amounts of the shale gas in each well. By using (1) and (2) results, the supply chain network, while meeting the freshwater demands in each well, determines (3) potential locations and transportation modes of freshwater supply, and wastewater treatment types, (4) drilling schedule in each site, total amount of shale gas production, transportation model of shale gas supply, and generation amount of electricity. This model is assessed from the case study of Marcellus shale play located in the United States. This study can help to identify the technological bottlenecks and major cost drivers for the strategy of the shale gas production considering the control of hydraulic fracturing system and can also be a guideline for the development of various mathematical programming models for the optimal design of the production of the shale gas in various potential plays.

Keywords: shale gas, hydraulic fracturing, water management

(22) Multiscale modeling and control of Kappa number and porosity in a batch pulp digester

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This work proposes a multiscale modeling and model-based feedback control framework for the delignification process in a batch-type pulp digester. Specifically, we focus on a hardwood chip in the digester and develop a multiscale model capturing both the evolution of microscopic properties such as the pore size and shape distributions in the solid phase, and the dynamic changes in the temperature and component concentrations in the liquor phase. While the macroscopic model adopts the continuum hypothesis based on the Purdue model, a novel microscopic model is developed via a kinetic Monte Carlo algorithm, accounting for the dissolution of lignin, cellulose and hemicellulose contacting the liquor phase. A reduced-order model was built to design a Luenberger observer for state estimation, which is then used to develop a model-based control system. The simulation results demonstrated that the proposed methodology was able to regulate both the Kappa number and porosity to desired values.

Keywords: Pulp digester, Pulp digester, Multiscale modeling

(23) Construction of a Semi-Stochastic Intracellular Signaling Model Via Global Sensitivity Analysis and Probability Density Estimation

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With recent advances in the ability to measure gene and protein expression at the single-cell level, it has been found that cells from a clonal population exhibit a large degree of cell-to-cell variability. Previous studies have applied stochastic modeling methodologies such as Gillespie's algorithm to simulate the single-cell dynamics. However, this method is often computationally expensive. Alternatively, a semi-stochastic modeling approach has been proposed. Specifically, a pre-specified probability density function (PDF) of the model parameters is used to generate different parameter values, which are subsequently used in the deterministic model to simulate corresponding distinct signaling dynamics. This approach allows simulation of cell-to-cell variability with a manageable computational cost. However, the PDF of the model parameters is usually unknown a priori as the model parameters are difficult to measure experimentally; therefore, the PDF needs to be inferred from measurements.

In this study, a sequential approach that consists of global sensitivity analysis, surrogate modeling, and probability density estimation is proposed to estimate the PDF of model parameters. First, a global sensitivity analysis method is used to identify a set of important model parameters. Second, a number of PDF of the identified parameters are sampled for generating the corresponding PDF of the outputs. These generated data then are used to develop a surrogate model to correlate the PDFs of the parameters and outputs. Next, the PDF of the identified parameters is estimated by minimizing the difference between the measured and predicted output PDF with the developed surrogate model. Through the proposed methodology, the parameter PDF can be inferred accurately, which can be used to construct a semi-stochastic model to identify the source of heterogeneity and to quantify their magnitude in the single-cell dynamics.

Keywords: Intracellular signaling pathway, mathematical modeling, probability density estimation

(24) Process Innovation Using Block Superstructure

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Process synthesis finds the best design alternatives among many other alternatives. A key point in process synthesis is to postulate feasible process alternatives and include the optimal candidate. Postulation of these alternatives is not intuitive. For instance, the design of a refrigeration cycle involves the challenges on equipment selection and connection. The discovery of such process alternatives often requires the analysis of phase diagrams embedding rich process information for conceptual process design. These design alternatives discovered through the thermodynamic diagrams are assembled as a superstructure for comprehensive analysis in process synthesis. However, analysis of these phase diagrams requires expert knowledge and a systematic approach for generating design alternatives is lacking when a new problem is encountered. In this work, we propose a new block-based superstructure enabling the systematic discovery and optimization of novel process flowsheets. The phase diagrams are described using a surrogate model for rigorous thermodynamic relation, e.g., Peng-Robinson equation of state, to reduce the computational complexity. The flowsheets will be screened among the rich connection information in the block superstructure with the surrogate thermodynamic relations. Unlike classic unit-based superstructure, the proposed block superstructure leverages on building blocks representing fundamental physiochemical phenomena. The block superstructure is constructed by assembling building blocks in a two-dimensional grid. These building blocks allow feed supplies and product withdrawing while connecting with each other through material and energy flow. We pose the process innovation problem as a mixed-integer nonlinear optimization (MINLP) problem. The objective is to find innovative flowsheet minimizing the total annual cost. We demonstrate the capability of the proposed approach through several case study on liquefied energy chain, refrigeration system.

Keywords: Process Synthesis, Process Intensification, Process Innovation

(25) Multilayer polymeric films on hollow fibers for light gas separation

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Energy remains a critical component in the separation of light gases (like hydrogen, carbon dioxide, nitrogen, methane). For a sustainable energy and fuel generation from coal, natural gas and biomass, low-cost and efficient separation remain a critical challenge. Till now, mainly exotic materials have been used as membranes for the separation process to provide higher selectivity of the desired gases like hydrogen. In contrast to these expensive exotic membranes, water-based polymers developed via layer by layer deposition of functional polymers on conventional Hollow fiber membrane system can be used to get a low cost, low-energy separation process.
Hollow fiber polymeric membrane employs high flux and a low production cost has been used as a substrate to provide a cost-effective solution to this problem. Layer-by-layer polymer coatings are formed by alternate deposition of positively and negatively charged polyelectrolytes. This work demonstrates a process through which hollow fibers can be used as a substrate for layer-by-layer deposition of functional polymers to provide high selective membranes for hydrogen/carbon dioxide separation.

Keywords: layer-by-layer assembly, membranes, hydrogen purification

(26) Tannic acid as a small molecule binder for silicon anodes in lithium-ion batteries

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[2] University of Ulsan

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Increasing demand for portable electronic devices, electric vehicles, and grid scale energy storage has spurred interest in developing high capacity rechargeable lithium ion batteries (LIBs). For this, researchers have been extensively studying materials with high lithium ion storage capability, especially silicon, to replace the graphite anode in LIBs. Silicon is a non-toxic, abundantly available material and has a theoretical gravimetric capacity of 3579 mAh/g with a low operating potential of 0-1 V vs. Li/Li+. However, silicon has not yet been commercialized as an anode material due to large volume variation (>300 %) during lithiation and delithiation which pulverizes silicon particles ultimately leading to battery failure. These problems can be overcome by using a binder that can hydrogen bond with the hydroxyl groups on silicon nanoparticles. Here, we demonstrate the use of tannic acid (TA), a natural polyphenol derived from wood, as a binder for silicon anodes in lithium ion batteries. The resultant silicon electrodes demonstrated decent cycling stability with a capacity of 1000 mAh/g for 200 cycles which can be attributed to the presence of abundant hydroxyl (OH) groups. Also, water processability makes the electrode synthesis process environmentally friendly. This work demonstrates that a molecule with numerous hydrogen bonding functional groups can be used a binder and that modifications in TA can further improve its performance as a binder in silicon anode.

Keywords: Hydrogen bonding, Tannic acid, Silicon anode

(27) An Integrated Data-Driven Modeling & Global Optimization Approach for Production Planning

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The tight competition, environmental regulations, and lower profit margins are some of the factors that drive the petrochemical industry to make planning and scheduling operations more efficient over the last few decades. Traditional production planning approaches rely on linear programming (LP) principles with fixed-yield planning models, even though refinery operations are nonlinear in nature. While there are commercially available models for simulation of processing units, such detailed models cannot be used in enterprise-wide approaches due to their high computational expense. Data-driven modeling, however, offers a promising way to obtain computationally inexpensive nonlinear models, which can relate relevant inputs to relevant outputs to describe each individual process accurately. In this work, we are proposing a framework for integrated data-driven modeling and global optimization to solve production planning problems to optimality. In the first step, we organize, analyze, and process the real plant data provided by Hyundai Oilbank's Daesan Refinery located in South Korea. Models of different complexities are trained, validated, and then compared to find the best data-driven model to describe each processes. In the second step of the work, we create a superstructure containing all possible connections and operating modes in the refinery. The resulting planning model is a multi-period planning non-convex nonlinear optimization model (NLP), which is solved to global optimality using commercial solvers. Several case studies are chosen to compare the optimal production plan with the actual one. Results of the case studies are provided to illustrate the efficiency of our proposed model and global optimization approach.

Keywords: petroleum refining, optimization, production planning

(28) Anti-oxidants unlock shelf-stable Ti3C2Tx (MXene) nanosheet dispersion

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[1] Artie McFerrin Department of Chemical Engineering, [2] Department of Material Science & Engineering

MXenes, such as Ti3C2Tx, are fascinating 2D nanomaterials with an attractive combination of functional properties suitable for applications such as batteries, supercapacitors, and strain sensors. However, fabrication of devices and functional coatings based on MXenes remains challenging as they oxidize and degrade quickly from reacting with water and dissolved oxygen. We examine oxidation of MXene nanosheets in various media (air, liquid, and solid) via multiple types of measurements to assess their shelf stability. The oxidation rate of MXene nanosheets were observed fastest in liquid media and slowest in solid media, and can be accelerated by exposure to UV light.

More importantly, we demonstrate an effective method to retard the oxidation of colloidal Ti3C2Tx MXene nanosheets by introducing antioxidants such as sodium L-ascorbate, ascorbic acid and tannic acid. The success of the method is evident in the stable morphology, less-changed structure, and colloidal stability of Ti3C2Tx. Even in the presence of water and oxygen, the electrical conductivity of Ti3C2Tx nanosheets treated with sodium L-ascorbate was orders of magnitude higher as compared to untreated ones after 21 days. The conductivity changes also reveal that the resistance to oxidation persists in the dehydrated MXenes as well. Our findings have the potential to be generalized to protect other types of MXenes as well and solve the most pressing challenge in the field of MXene engineering.

Keywords: MXene, 2D nanomaterials, Anti-oxidation

(29) Systematic Analysis, Design and Optimization of Water-Energy Nexus

Spyridon Tsolas[1], M. Nazmul Karim[1], M. M. Faruque Hasan[1]

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Securing scarce energy and water resources from the environment, while at the same time satisfying on-growing water and energy demands for end-use consumption is crucial. The intermediate processing facilities, energy sources (acting also as water sinks) and water sources (acting as energy sinks), receive energy and water natural resources respectively, process, exchange and deliver them as usable electricity, fuels and water for consumption. It is important to quantify the performance of this water-energy nexus, and understand how it is affected by the different processing technologies, operating capacities and their connectivity.

To this end, we present a scalable, graph-theoretic representation of a nexus for the design and optimization of complex water-energy systems. We define a nexus as a directed bipartite graph with water and energy flows and show that for specified external grid demands, the optimal nexus configuration with minimum water and energy generation is the one without any redundant subgraphs. We then introduce the water-energy (WEN) diagram that can systematically identify and eliminate those redundant subsystems. This leads to (i) minimum generation/extraction of water and energy resources from the environment, or (ii) maximum yield of water and energy to meet external demands. In the second part, we develop a superstructure mathematical programming-based algebraic method that provides the same results but for more complicated and large-scale nexus design. This also takes into account the intensity factors of the sources, restrictions on source-sink matching, and quality specifications. The model is further extended to include capital and operating costs of the processing facilities, as well as geographic distances. The approach is demonstrated using case studies on water-energy nexus systems at regional and national scales.

Keywords: Sustainable energy and water planning, Water-energy nexus, Water-energy supply chain

(30) Magnetically driven functionalized nanoplatelets Pickering emulsion for removal of oil contaminants from water

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There is an immense need for efficient cleanup and recovery of industrial grade oil in today's society. Incidents like the BP Deepwater Horizon oil rig explosion in the Gulf of Mexico in 2010 and Sanchi tanker collision in East China Sea in Jan. 2018 have caused huge oil spill and tremendous harm to the environment. This has resulted in the loss of billions of dollars due to the loss of products and cleanup efforts, which now has drawn considerable attentions for the environmental merits. The purpose of our research is to develop an effective and inexpensive method to absorb crude oil from oil-water mixtures. Functional magnetic nanoplatelets can be designed as Pickering emulsion surfactant for targeting removal oil contaminants from seawater. After introducing magnetic nanoparticles into water-oil mixtures, small oil droplets will be stabilized by two-dimensional Pickering nanoemulsifier and can be easily controlled to move by the external magnetic field. The advantage of utilizing magnetic particles to extract oil droplets from mixture is that oil droplets can move as designed direction and easily be reclaimed for use. Small stable oil droplets are relatively hard to remove and costly, but adding magnetic nanoparticles and establishing an application with magnetic field can restore large amount of extracted oil with a high speed. This magnetic particle approach can be considered as an environmental and promising technology for oil water separation.

Keywords: 2D nanoplatelets, oil-water separation, magnetic driven

(31) Engineering Design and Optimization of Protein Transformation into Bacterial Cells

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Electroporation of purified proteins and internalization into bacterial cells has been employed in the past to introduce fluorescently-labeled target proteins into the cytoplasm. This enables the use of powerful fusions with fluorescent dyes that exhibits superior signal-to-noise ratio and long-lived fluorescence output compared to fluorescent proteins. Here, we employed standard engineering design techniques to develop a multi-parameter model in order to optimize the transformation, motility and viability of the transformed cells. Systematic experiments were carried out to determine the yield, defined in terms of the fraction of transformed cells in a population, and the viability, over varying concentrations of cells, proteins, buffer systems for proteins, as well as electric field strengths. I will discuss the nature of the correlations between cell viability, motility and the transformation yield at a single cell and population level. I will also discuss strategies to obtain the best possible yield including different transformation techniques. . Purified eYFP was employed to study the transformation. Important parameters for optimization included protein, cell concentrations, buffer systems for protein, and the electric field strengths. Yield was determined by quantitative analysis of single cell intensities when transformed with the purified fluorescent product.

It is anticipated that our work will help the design of robust protein transformation strategies.

Keywords: Bioengineering, electroporation, protein purification

(32) Towards the incorporation of operability and safety in the synthesis of intensified reactive and extractive separation systems

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Intensified processes typically feature higher degree of integration of multifunctional phenomena, less degrees of freedom, narrower operability windows, and even faster dynamics. Thus, the incorporation of control, operability, and safety assessment at the design level becomes even more critical to ensure the actual operational performances in these systems, comparing to their conventional unit-operation-based counterparts. Despite recent advances, systematic synthesis approaches and analytical tools for the design and operability/safety optimization of intensification processes are still lacking.

To address this challenge, in this work we propose a systematic framework for the synthesis of operable process intensification systems, with specific focus on reactive and extractive separation processes. This framework is based on a phenomenological process intensification/synthesis approach (i.e., Generalized Modular Representation Framework (GMF)), which first identifies candidate/promising intensified tasks and then translates them to equipment-based flowsheet alternatives. Flexibility analysis is integrated with the GMF model to ensure that resulting design configurations can be operable under varying operating conditions. To systematically account for inherent safety performance, risk assessment criteria are included as process constraints considering failure frequency and consequence severity. Simultaneous design and control strategies are also employed to ensure validated operable intensified design configurations using advanced multi-parametric model- based predictive control (mp-MPC) developed via the PAROC (i.e., PARametric Optimization and Control) framework. Two case studies are presented to highlight the potential of the proposed approach: (i) a reactive separation system - methyl-tert-butyl-ether production, and (ii) an extractive separation system - methanol/water azeotropic separation.

Keywords: Process intensification, Process synthesis, Process operability/safety

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A. ORAL PRESENTERS

i) MORNING SESSION

1. Rapid One-Pot Microwave Synthesis of Mixed Linker Hybrid Zeolitic-Imidazolate Framework Membranes for Tunable Gas Separations

Febrian Hillman[1], Jordan Brito[1], and Hae-Kwon Jeong[1,2]

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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. Furthermore, the slow fabrication of MOF membranes restricts their commercialization. Studies have shown that through mixing linkers, one can continuously tune the ZIFs (termed hybrid ZIFs) properties to match with the characteristic of specific gas mixture.

Herein we report a rapid one-step microwave-assisted synthesis of mixed linker ZIF-7-8 membranes in under ~ 90 seconds. ZIF-7-8 consists of Zn2+ metal nodes bridged by a mixture of benzimidazolate (bIm, ZIF-7 linker) and 2-methylimidazolate (mIm, ZIF-8 linker) linkers. To the best of our knowledge, this is the fastest synthesis of any polycrystalline MOF membranes reported up to now. Furthermore, the gas separation performances (separation factor and permeance) of hybrid ZIF-7-8 membranes were systematically tuned by varying the bIm-to-mIm ratio incorporated into the framework. The unprecedentedly rapid synthesis of ZIF-7-8 membranes with tunable molecular sieving properties is an important step.

2. Micro-encapsulation with Nanoplatelet Surfactant

L. Eric Zhang[1,2] and Zhengdong Cheng[1,2]

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

Abstract:

We demonstrated the possibility to employ both microfluidics and Janus nanopletes to fabricate capsules at micrometer level. Conventional encapsulation technologies apply polymer material as shell structure, which complicates the manufacturing procedure and increases cost of micro capsules. In our work, utilizing the Janus nanoplatelet surfactant developed in our lab, we are able to simplify the encapsulation procedure by integrating the shell material and the emulsifier. The geometry of the capsule comprises a layer of Janus platelet shell, a swellable hydrogel core and encapsulated active ingredient. During the manufacturing the Janus platelet can serve as an emulsion stabilizer and the precursor of the shell structure. With a coaxial microfluidics device, we are able to encapsulate hydrogel and water soluble active ingredients with the Janus nanoplatelet surfactant, and then polymerize the capsules with UV-initiator. The release of active ingredients can be controlled by hydrogel swelling. Several applications with this technique are demonstrated. Such a Janus particle microencapsulation technique has a potential to be applied in biomedical, cosmetic and oil & gas industry.

3. Multifunctional Charge Transfer-Based Supramolecular Materials with Tunable Thermochromism

Tianyu (Kelvin) Yuan[1], Lei Fang[1, 3], and Mark A. Olson[2]

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Abstract:

Stimuli-responsive materials, such as thermochromics, have found mass usage and profitability in manufacturing and process control. Imparting charge transfer-based functional supramolecular materials with tunable thermochromism, emerges as an ideal strategy to construct optically responsive multifunctional assemblies. A new series of thermochromic charge transfer-based supramolecular materials assembled in water has been developed. These assemblies are composed of a bis-bipyridinium-derived acceptor and a series of commercially available donors – namely, the neurotransmitter melatonin and its analogue bioisosteres. By tailoring the chemical structure of the donors, the strength of the charge transfer interactions can be tuned. Thermochromic aerogels and inks of these materials are prepared, with a large selection of colors, in environment-friendly solvents and demonstrate tunable thermochromic transition temperatures ranging from 45 to 105 °C. Stamped and inkjet-printed thermochromic patterns can be prepared from their aqueous solutions which also showed favorable compatibility with commercial inks. Mechanistic studies reveal that the two types of water molecules were bound to the supramolecular complexes with different strength, and the more weakly bound water is responsible for the thermochromic transitions.
Overall, this work presents a novel series of donor-acceptor CT-based supramolecular materials which feature versatile processability and tunable thermochromic properties. The unfolded design principles and underlining mechanism in this work provide essential insights for the future development of reversible and recyclable thermochromic supramolecular materials.

4. Relative Abundance of *Candida Albicans* and *Candida Glabrata* in *In Vitro* Co-culture Biofilms Impacts Biofilm Structure and Formation

Michelle L. Olson, Arul Jayaraman, and Katy C. Kao

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

Abstract:

Candida is a member of the normal human microbiota and often resides on mucosal surfaces such as the oral cavity or the gastrointestinal tract. In addition to their commensality, *Candida* species can opportunistically become pathogenic if the host microbiota is disrupted or if the host immune system becomes compromised. An important factor for *Candida* pathogenesis is its ability to form biofilm communities. The two most medically important species - *Candida albicans* and *Candida glabrata* - are often co-isolated from infection sites, suggesting the importance of *Candida* co-culture biofilms. In this work, we report that biofilm formation of the co-culture population depends on the relative ratio of starting cell concentrations of *C. albicans* (Ca) and *C. glabrata* (Cg). When using a starting ratio of Ca:Cg of 1:3, a ~6.5- and ~2.5-fold increase in biofilm biomass was observed relative to Ca monoculture and a Ca:Cg ratio of 1:1, respectively. Confocal microscopy analysis revealed heterogeneity and complex structures composed of long Ca hyphae and Cg cell clusters in the co-culture biofilms, and qRT-PCR studies showed an increase in the relative expression of the *HWP1* and *ALS3* adhesion genes in the Ca:Cg 1:3 biofilm compared to Ca monoculture biofilm. Additionally, only the 1:3 Ca:Cg biofilm demonstrated increased resistance to the antifungal drug caspofungin. Overall, the results suggest that interspecific interactions between these two fungal pathogens increase biofilm formation and virulence-related gene expression in a co-culture composition-dependent manner.

5. Modulation of Ultrasensitive Signaling in Bacteria by Viscous Load on Flagellar Motor

Jyot Antani and Pushkar Lele

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

Abstract:

Mechanical forces are known to influence signaling in several biological systems. In recent years, several mechanosensitive proteins have been implicated in bacterial colonization and pathogenesis. Our earlier work showed that the bacterial flagellum, an appendage that enables motility, is an adaptive mechanosensor (Lele et al., PNAS, 2013). Recent results from our lab suggest that the mechanosensitive force-generators within the flagellar motor are activated through a catch-bond type mechanism (Chawla et al., Sci Rep, 2017). We have found additional mechanosensitive functions of the flagellar motor: a molecular flagellar switch, which enables reversals between clockwise (CW) and counterclockwise (CCW) directions of rotation, is also modulated by mechanical signals. This modulation is likely important for chemotaxis and bacterial swarming (Lele et al., Sci Adv, 2016), but the molecular mechanisms remain unknown. Here, we determined how viscous loads (mechanical forces) modulate the activity of the flagellar switch by controlling its ultrasensitive response to an allosteric response regulator, CheY-P. We employed the popular tethered-bead assays as well as tethered cell techniques to apply varying magnitudes of viscous loads on individual motors. Next, we measured the switch activities in a large population of cells and employed a statistical distribution technique to determine the dose-response relations (CW_{bias}-[CheY-P]) as a function of load. Our preliminary observations suggest that modulation either occurs through the control of the flagellar switch structure or via the mechanosensitive response of stator-units involved in motor rotation.

6. Stochastic Modeling of CTB-GM1 Binding Kinetics

Dongheon Lee[1,2], Alec Mohr[1], Joseph S. Kwon[1,2], and Hung-Jen Wu[1]

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Abstract:

Cholera toxin (CTx) is a toxin protein, which can lead to lethal cholera. CTx is an AB_5 protein that consists of an enzymatic A-subunit and five identical cholera toxin B-subunits (CTB). CTB binds with gangliosides such as GM1 on host cell membrane, which facilitates the endocytosis of CTx and the development of cholera. How cholera toxin subunit B (CTB) binds to its receptor on host cell membrane is still not fully understood due to its complex nature. Since the binding events highly depend on the current surface configuration, the kinetic Monte Carlo methodology is applied to simulate the complex interactions between CTB and GM1 microscopically. The proposed kMC model considers receptor migration, CTB attachment and detachment, and surface forward and backward reactions as discrete microscopic events. At every moment, an event to be executed is selected randomly based on the rates of all possible events, and this procedure continues till the end of simulation. In summary, we utilize theoretical modeling to explore cholera pathogenesis and offers a systematic tool for the biomedical community to reveal the pathogenesis of other diseases.

7. Optimal Design of Energy Systems using Constrained Grey-Box Multi-objective Optimization

Burcu Beykal[1,2], Fani Boukouvala[3], Christodoulos A. Floudas[1,2], and Efstratios N. Pistikopoulos[1,2]

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Abstract:

The (global) optimization of energy systems, commonly characterized by high-fidelity and large-scale complex models, poses a formidable challenge partially due to the high noise and/or computational expense associated with the calculation of derivatives. This complexity is further amplified in the presence of multiple conflicting objectives, for which the goal is to generate trade-off compromise solutions, commonly known as *Pareto-optimal* solutions. We have previously introduced the p-ARGONAUT system,

parallel AlgoRithms for Global Optimization of coNstrAined grey-box compUTational problems, which is designed to optimize general constrained single objective grey-box problems by postulating accurate and tractable surrogate formulations for all unknown equations in a computationally efficient manner. In this work, we extend p-ARGONAUT towards multi-objective optimization problems and test the performance of the framework, both in terms of accuracy and consistency, under many equality constraints. Computational results are reported for a number of benchmark multi-objective problems and a case study of an energy market design problem for a commercial building, while the performance of the framework is compared with other derivative-free optimization solvers.

8. Integration of Design, Scheduling, and Control of Combined Heat and Power Systems: A Multiparametric Programming Based Approach

Baris Burnak[1,2], Justin Katz[1,2], Nikolaos A. Diangelakis[2], and Efstratios N. Pistikopoulos[1,2]

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Abstract:

The operation of multiproduct/multipurpose processes involves decisions at different time scales; such as short-term for control, medium-term for scheduling, and long(er)-term for design. At all these scales, uncertainty plays a key role with fluctuations in product demand, prices, availability of units, as well as raw materials and product specifications. While it has been widely accepted that simultaneous decision making at these three layers are expected to deliver cost-effective and intensified/integrated processes; such an integration still poses formidable challenges due to the order of magnitude differences in the time-scale, the often-conflicting objectives at the different layers, etc. However, recent advances in this area provide a sound basis for further development.

In this work, we present a unified framework towards this direction for the case of multiproduct/multipurpose processes. Based on the PAROC (PARametric Optimization and Control) framework featuring (i) a single high-fidelity model, (ii) multi-parametric Rolling Horizon Optimization (mpRHO) policies to readjust for the changing market structures, (iii) multi-parametric Model Predictive Control (mpMPC) for efficient set point tracking and, (iv) a surrogate model formulation to bridge the time gap between mpRHO and mpMPC, we derive (i) design dependent and scheduling aware control strategies, and (ii) scheduling strategies that are design dependent and control aware. The multi-parametric formulation of the integrated scheduling and control schemes yields offline maps of optimal actions that enable design and operational optimization under uncertainty. The framework is illustrated on a combined heat and power (CHP) system, involving two CHPs operating in tandem to satisfy the time-variant heat and electricity demand from multiple residential units. We utilize the proposed methodology to simultaneously determine (i) the optimal size of the internal combustion engine, (ii) the decentralized control schemes for different operating policies, and (iii) the coordination of the parallel operations of the CHP units.

9. Simultaneous Process Network Synthesis and Process Intensification Using Block Superstructure

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

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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. Current optimization-based process synthesis methods are unable to automatically construct and identify novel intensified equipment 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 block-based superstructure instead of classical unit-operation based one. Each block represents a unit use of materials with a specific function (reaction, separation, storage). The existence of connecting streams between adjacent blocks and jump flows among all blocks enables the necessary interactions between different blocks via material and energy flows. 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.

10. Adsorption of Carbon on Partially Oxidized Cu Surfaces - Applications to Graphene Synthesis

Behnaz Rahmani Didar and Perla B. Balbuena

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Abstract:

Currently, the Catalytic Chemical Vapor Deposition is the most popular method for the synthesis of graphene and carbon nanotubes. Copper (Cu) as the catalyst in this process has shown much potential for growing high quality fragments of graphene. Experimentally, it has been observed that predosing Cu substrates with oxygen before graphene growth has a cleaning effect on the substrate. We study and discuss this process using DFT on two surfaces of Cu; (100) and (111).Our results show that on both surfaces, an incoming carbon atom has the ability to replace and completely desorb a previously surface-adsorbed oxygen atom producing CO and CO_2 molecules in the gas phase. By comparison, the (111) surface is better suited for oxygen desorption, and an incoming carbon atom can more easily bond to and desorb oxygen atoms even at low oxygen coverages. We also examine this mechanism at two different temperatures for both surfaces at 0.5 ML oxygen coverage.
Our results in this study shows first-principles evidence of the cleaning effect of oxygen on Cu surfaces in the presence of carbon with applications to graphene and carbon nanotubes synthesis. Conversely, adsorption and diffusion of carbon atoms, both of which are necessary for the nucleation and growth of carbon nanotubes, may be hindered by the presence of the oxidized or partially oxidized surfaces. Such desorption of carbon as CO or CO_2 in partially or totally oxygenated surfaces may be one of the reasons for the undesired termination of carbon nanotube growth.

11. Calorimetric Study of Graphene Oxide Thermal Stability

Pritishma Lakhe[1], Devon Kulhanek[2], Wanmei Sun[2], Bin Zhang[1], Micah J. Green[2], and M. Sam Mannan[1]

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Abstract:

Large-scale production of graphene is of increasing commercial and academic interest because graphene has shown immense potential in energy storage and composite filler applications. Synthesis routes that involve graphene oxide (GO) are predominantly used because this method has shown potential for bulk production at high yield. This method involves the oxidation of graphite to GO and its subsequent reduction to reduced graphene oxide (rGO). However, prior studies have shown that GO can undergo explosive decomposition under certain conditions. There is no documented process safety incident related to GO so far, but GO is an energetic material that can undergo explosive thermal reduction. The motivation of this research is to investigate potential process safety issues with bulk GO storage and handling because the industry is ramping up large-scale manufacturing of GO. Our data shows increasing GO mass decreases the temperature at which material decomposes. We quantified the pressure release rate and pressure generation during decomposition. We also discussed the underlying causes of the explosive behavior of bulk GO and proposed safer storage and handling conditions. Studies were conducted in Advanced Reactive System Screen Tool (ARSST). We compared the GO decomposition made in lab using modified Hummers method to the commercially available GO. Finally, we used the Frank Kamenetskii model to obtain the critical density and mass necessary for GO decomposition. This research will be beneficial in assessing the hazards of GO and enhancing the safety of rGO production processes over their life cycles.

12. Toward Optimal Synthesis of Renewable Ammonia and Methanol Processes

C. Doga Demirhan[1,2], William W. Tso[1,2], and Efstratios N. Pistikopoulos[1,2]

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Abstract:

The conversion and storage of renewables into useful and transportable energy vectors is an outstanding challenge in transitioning to a sustainable energy future. Ammonia and methanol are two promising vectors due to their proven production and transportation infrastructures. Individual processes consuming fossil fuels have been improved and optimized over the years, but there is no clear path forward for incorporating renewables or their coproduction. In this work, we introduce a deterministic global optimization-based process synthesis framework to determine the minimal cost for the coproduction of ammonia and methanol from hardwood biomass and natural gas. This will provide the guideline for future studies into solar and wind energy. A process superstructure with several competing technologies and integration routes is modeled and described. A customized branch-and-bound algorithm is used to solve the resulting mixed-integer nonlinear nonconvex optimization model. Results indicate that the biomass incorporated processes are cost-competitive with pure fossil fuel based processes, and the integration of ammonia and methanol production leads to 4-7% savings.

ii) AFTERNOON SESSION

13. Surface-Agnoistic Highly Stretchable and Bendable Conductive MXene Multilayers

Hyosung An[1], Touseef Habib[1], Smit Shah[1], Huili Gao[2], Miladin Radovic[2,3], Micah J. Green[1,3], and Jodie L. Lutkenhaus[1,3]

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Abstract:

Stretchable, bendable, and foldable conductive coatings are crucial for wearable electronics and biometric sensors. Such coatings should maintain functionality while simultaneously interfacing with different types of surfaces undergoing mechanical deformation. MXene sheets as conductive 2D nanomaterials are promising for this purpose, but it is still extremely difficult to form surface-agnostic MXene coatings that can withstand extreme mechanical deformation. Herein, we demonstrate conductive and conformal MXene multilayer coatings that can undergo large-scale mechanical deformation while maintaining a conductivity as high as 2000 S/m. MXene multilayers are successfully deposited onto flexible polymer sheet, stretchable poly(dimethylsiloxane), nylon fiber, glass, and silicon. The coating shows a recoverable resistance response to bending (up to 2.5 mm bending radius) and stretching (up to 40% tensile strain). We demonstrated that the MXene multilayer films could be used as strain sensors to topographically sense objects or materials deformation.

14. 3D Graphene Oxide Gel Assembly: Effects of Nanosheet Morphology and Ammonia on Gel Properties and their use as Structural Electrodes for Energy Storage

Smit A. Shah[1], Dorsa Parviz[2], Morgan G. Odom[3], Wanmei Sun[1], Devon Kulhanek[1], and Micah J. Green[1,3]

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Abstract:

3D graphene oxide (GO) based gels synthesized using sol-gel technique have gained remarkable interest because of their ability to retain individual nanosheet properties. The high specific surface area and electrical conductivity of these 3D gel networks makes them suitable active material for electrochemical energy storage applications. However, 3D GO gel's electrical conductivity, surface area and density depend on the crosslink type and density. Here we investigate the role of ammonia and precursor nanosheet morphology on the crosslink type and density of 3D GO gels. Our results indicate that ammonia strongly affects the formation of inter-sheet bridging structures as well as the deoxygenation and reduction of nanosheets during gelation. Thermal annealing of GO gels result in an increase in their electrical conductivity and displacement of nitrogen. We also altered the GO nanosheet morphology to obtain crumpled GO (CGO) nanosheets and prepared 3D aerogels with mixtures of GO-CGO nanosheet dispersions. The properties of these gels demonstrate how the GO morphology can allow for an additional handle in creating GO-based gels with tunable density, electrical conductivity, and surface area. We investigated the composites of GO gel with aramid nanofibers (ANFs) to obtain improved mechanical properties for their application as structural supercapacitor electrodes.

15. High Efficient Oil-Water Separation using Surface-Programmable Membranes

Glenn Zeng[1], Lecheng Zhang[1], Dali Huang[2], and Zhengdong Cheng[1,2]

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[2]*Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843*

Abstract:

The challenge of separating emulsified oil from water has sparked enormous research interests in developing advanced membrane technology. One of the most crucial elements to achieve high separating efficiency lies in the design of interfacial structure of membranes. Herein, we present a surface-programmable membrane for separating oil-water emulsions. Owing to the precise control on the surface chemistry of membranes, the hybrid membrane not only separates the oil-water mixture with high efficiency (>99.2%), but also demonstrates high versatility for many advanced applications, e.g., self-healing and heavy metal removal. This research opens up new opportunities in developing multifunctional membrane-based materials.

16. Synthetic, Functional Thymidine-Derived Polydeoxyribonucleotide Analogues from a Six-Membered Cyclic Phosphoester

Yi-Yun Timothy Tsao[1-3], Travis H. Smith[1-3], and Karen L. Wooley[1-3]

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Abstract:

A grand challenge that crosses synthetic chemistry and biology is the scalable production of functional analogues of biomacromolecules. We have focused our attention on the use of deoxynucleoside building blocks bearing non-natural bases to develop a synthetic methodology that allows for the construction of high molecular weight deoxynucleotide polymers. Our six-membered cyclic phosphoester ring-opening polymerization strategy will be demonstrated, by an initial preparation of novel polyphosphoesters, comprised of butenyl-functionalized deoxyribonucleoside repeat units, connected *via* 3',5'-backbone linkages. Computational modeling of the six-membered 3',5'-cyclic phosphoester ring derived from deoxyribose indicated strain energies at least 5.4 kcal/mol higher than the six-membered monocyclic phosphoester. These calculations supported the hypothesis that the strained 3',5'-cyclic monomer can promote ring-opening polymerization to afford the resulting polymers with low dispersities. Regioregularity is a crucial property in the synthesis of DNA analogues, as natural DNA is synthesized exclusively in the 5' to 3' direction. The regioisomeric preference was investigated by comparison to synthesized model compounds of 3',3'-, 3',5'-, and 5',5'-linkages. 31P NMR spectra revealed the major connectivity in the polymer backbone to be 3',5'-linkages, with ≤30% of other isomeric forms. Model reactions employing a series of alcohol initiators imparting various degrees of steric hindrance were then conducted to afford the corresponding ring-opened unimer adducts and to gain understanding of the regioselectivity during the ring-opening polymerization. 1H−31P heteronuclear multiple-bond correlation spectroscopy showed ethanol and 4-methoxybenzyl alcohol initiation to yield only the P−O5' bond cleavage product, whereas attack by isopropyl alcohol afforded both P−O3' and P−O5' bond cleavage products, supporting our hypothesis that the increased steric hindrance of the propagating species dictates the regioselectivity of the P−O bond cleavage. Overall, this work provides a fundamental understanding of the polymerization behavior of six-membered cyclic phosphoesters and broadens the scope of DNA analogues from the ring-opening polymerization of 3',5'-cyclic phosphoesters.

17. Polymer-Clay Nanocomposite Coatings as Efficient, Environment-Friendly Surface Pretreatments for Aluminum Alloy 2024-T3

Pilar C. Suarez-Martinez[1], Jerome Robinson[2], Hyosung An[1], Robert C. Nahas[2], Douglas Cinoman[2], and Jodie L. Lutkenhaus[1]

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Abstract:

Surface pretreatment coatings are a research area in continuous transformation. Moving away from the well-known chromium conversion coatings (CCC) toward an environment-friendly alternative is of great interest. Materials such as the aluminum alloy 2024-T3 (AA2024-T3) used in aircraft, for example, provide good mechanical performance but lack good corrosion resistance. Here, we present a polymer-clay coating made from branched polyethylenimine (BPEI) and montmorillonite (MMT) clay as a potential CCC substitute, and we examine this for the corrosion protection of AA2024-T3. This polymer-clay coating is applied by airbrushing an aqueous BPEI/MMT mixture onto any substrate. With this approach, application time is significantly reduced in comparison to other techniques (e.g. layer-by-layer assembly), and the structure of the polymer-clay coating is finely tuned by controlling the polymer-clay ratio. Results from electrochemical measurements and salt spray testing reveal good long-term (40d) corrosion protection of AA2024-T3 provided by a 1.8 μm thick coating with a 20:80 polymer-clay ratio. This polymer-clay ratio yields a highly ordered multilayered brick and mortar structure, where MMT (bricks) provides a physical barrier for the diffusion of corrosive agents/corrosion products within the coating, and BPEI (mortar) provides structural support and decelerates the corrosion process through surface buffering.

18. Water and Ion Pairing Universally Influence the Glass Transition of Polyelectrolyte Complexes

Yanpu Zhang[1], Piotr Batys[2,4], Joshua T O'Neal[2], Fei Li[1], Maria Sammalkorpi[3], and Jodie L. Lutkenhaus[1,2]

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Abstract:

The glass transition of a polyelectrolyte complex is long known to be influenced by hydration and salt doping. For example, it is generally accepted that increasing water content or salt doping depresses the glass transition temperature (T_g). However, there lacks a quantitative and physically meaningful relationship among these parameters that captures the behavior across more than one polyelectrolyte complex system. Here, modulated differential scanning calorimetry and all-atom molecular dynamic simulations are cooperatively exploited to investigate complexes paired from poly(diallyldimethylammonium chloride) and poly(sodium 4-styrenesulfonate). This relationship reveals that the glass transition is quantitatively controlled by the number of water molecules surrounding polyelectrolyte-polyelectrolyte ion pairs. Because this relationship also holds for another different polyelectrolyte complex system, it suggests that it might be considered "universal". Simulations reveal the extent of water clustering around different types of ion pairs during the glass transition process. These results explain broadly the fundamental - but nontraditional - plasticization influence of water, which impacts current interpretations of PECs for humidity annealing, temperature-responsive platforms, swelling, and sensing for a wide range of applications.

19. Shale Gas Techno-economic Analysis: Designing Separation Units to Handle Feedstock Variability

Eric Bohac[1], Mahmoud El-Halwagi[1], and Debalina Sengupta[2]

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[2]*The Gas and Fuels Research Center, Texas A&M Engineering Experiment Station, College Station, TX 77843*

Abstract:

One of the key challenges with shale gas is the wide variability in its composition and flow rate. The composition and flow rate, both between wells, and within the same well over time, can differ significantly. This is a challenge when designing a plant of optimal size. In general plants with larger process equipment are more flexible, and are able to handle a wider range of inlet compositions, however these plants also have higher fixed and operating costs.

In this work compositional variability is considered when designing a dehydration, NGL recovery, and fractionation train facility for a plant with a fixed inlet flowrate. A range of compositions are considered known. Conventional technology is used A plant is then designed for this base case process and is then simulated using ProMax, and fixed and variable costs are estimated using Aspen Process Economic Analyzer. Next five other cases representing the range of wellhead compositions in this region are run through the base case process design, assuming the same inlet flowrate, and any needed process modifications are made. Then revenue from the sale of shale gas and NGLs are compared with the additional fixed and variable costs for each case. The determination is then made based on process economics whether each case is worth treating or not. Safety impacts of the various cases are also considered, as is an additional case with a high acid gas content.

20. Model Approximation in Multiparametric Optimization and Control – A Computational Study

Justin Katz[1,2] , Nikolaos A. Diangelakis[2], and Efstratios N. Pistikopoulos[1,2]

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Abstract:

The development of a high fidelity model to accurately describe a dynamical system can lead to a complex structure of (partial) differential algebraic equations. Incorporating these highly complex, coupled, and nonlinear systems into optimization and control studies may often lead to an intractable problem. Reduction of such large scale systems into more tractable forms is typically done via model approximation; for example in control studies some form of linearization or complexity reduction is performed. Such model approximations are also at the heart of the Parametric Optimization and Control (PAROC) framework for the derivation of explicit/multiparametric controllers and/or online (e.g. MPC) explicit strategies. A key question that remains open within the PAROC framework is *what constitutes a suitable approximate model for the derivation of explicit control strategies with multiparametric programming*?".

In this work, we present a computational study towards addressing this question. In particular, we study system identification, and piece-wise linearization, in order to gain fundamental insights on the impact of the model approximation on (i) the solution of the multiparametric optimization problem, and (ii) the derived explicit control strategies. A computation study which features a detailed comparison based on error metrics is proposed in the following steps. Open loop dynamic optimization is first performed on a variety of high fidelity models of increasing complexity to ascertain the `desired' optimal trajectories. These optimal trajectories are then compared to the trajectories determined from advanced control strategies, including explicit/multiparametric MPC, which are based on model approximations. Key error metrics include model accuracy, controller accuracy, and deviations from the `desired' optimal trajectory. Two systems are used as a basis for this computational study: (i) a linear tank system with minimal complexity utilized to highlight the main principles of this approach, and (ii) a CSTR system where the reaction mechanisms are manipulated to increase the model complexity.

21. Systematic Analysis and Optimization of Water-Energy Nexus

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

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Abstract:

We present a scalable and systematic method for the design and optimization of complex water-energy nexus using graph theory-based network representation and a novel water-energy nexus (WEN) diagram. The graph-theoretic approach defines a nexus as a directed bipartite graph with two product flows, namely water and energy. The network representation allows decomposing a complex nexus into essential and redundant components. We show that for specified external grid demands, the optimal nexus configuration with minimum generation is the one without any redundant subgraphs with closed cycles. We then propose a systematic method to identify and eliminate redundant cycles, flows and entities within a nexus leading to (i) minimum generation/extraction of water and energy resources from the environment, or (ii) maximum yield of water and energy to meet external demands. Our proposed graphical approach is simple to implement and results in optimal nexus configurations. The approach is demonstrated using case studies on national and regional water-energy systems.

22. Improved Flare Radiation Criteria in Terms of Solar Radiation Contribution

Ankita Taneja[1], Delphine Laboureur[1,2], Bin Zhang[1], and M. Sam Mannan[1]

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

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Abstract:

At chemical processing plants, a flare stack is used to get rid of unwanted or excessive gases and relieve the system of excess pressure by combustion, thus causing high heat to radiate to atmosphere. Heat radiated from flare is important for siting flare at a proper location. The heat radiation should not exceed recommended threshold level so that people on-site and the equipment are not affected. Thus, to have a well-designed flare, knowledge of total radiation emitted from a flare is important to know. It will aid in accurately estimating the flare height and the area near the flare which would sustain high level of thermal radiation.
A common point of contention while calculating radiation level emitted from flare is the decision of including solar radiation (SR) in the calculations. API 521 mentions it to be discretionary upon the flare design company. However, some literature states that for all practical purposes, solar radiation contribution can be discounted.
The work performed aims at presenting a framework which quantitatively addresses aforementioned obscurity. The analysis helps flare designers to more objectively decide whether to include SR or treat it insignificant. The work studies the factors that cause variation in SR value: location, time, and orientation of the surface. Considering all these parameters, an appropriate value of SR is chosen to be the contribution of Sun to thermal radiation from flare. The effect of SR to design of flare is quantified by studying the change in effect distance near the flare and the height of flare. Consequence analysis software PHAST is used to obtain these calculations. In addition, the outcome that SR inclusion will have on the risk posed by the flare due to thermal radiation on personnel is also examined. This is studied by measuring the change in lethality and heat stress caused by radiation exposure.

23. Predicting Influence of Packing Shape and Loading Methodology upon Fixed-bed Structures

Srikanth Panyaram and Benjamin Wilhite

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Abstract:

Fixed beds are ubiquitous in chemical industry, finding use for gas-solid, liquid-solid, gas-liquid solid catalytic as well as gas-liquid mass transfer processes (absorption, distillation). The local packing structure of the fixed-bed provides surface area for fluid mass transfer, house catalyst material for reactions and dictates local flow patterns. Heterogeneities in packing configurations may result in increased pressure drop, fluid maldistribution and/or under-utilization of catalyst material, making an understanding of packed-bed structure essential to the efficient operation of these units.

Bed-packing algorithms have been developed for generating detailed three-dimensional maps of local bed structure. The algorithm has been tailored to study two widely used shapes in industry; spheres and cylinders. The study provides important insights into the global and local properties of the fixed-bed as a function of particle size, shape and loading methodology. Shape and size distribution of the particle sample influences the global and radial voidage. An essential component of this study is to understand how loading methods can influence the evolution of the properties exhibited by the beds. Different loading methods have been used to study the influence of particle-particle and particle-wall interactions. These interactions have shown to influence the voidage and orientation effects within the packing structures. Finally, the effect of these parameters on the evolution of fluid flows in fixed beds is elucidated. These investigations help in developing tools to manipulate the heterogeneities in packed beds to enhance reactor performance.

24. A Sustainable Process Design Approach for On-purpose Propylene Production and Intensification

Ashwin Agarwal[1], Debalina Sengupta[2], and Mahmoud M. El-Halwagi[1,2]

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[2]*The Gas and Fuels Research Center, Texas A&M Engineering Experiment Station, College Station, TX 77843*

Abstract:

The advent of Shale Gas and the increasing spread between the supply and demand curves for propylene present an opportunity for adopting alternative pathways to produce propylene. This study aims to investigate a sustainable process design approach to on-purpose propylene production. A hierarchical approach to sustainable process design is proposed and implemented in a case study. An initial evaluation of different propylene production technologies yielded propane dehydrogenation (PDH) as the most profitable route and hence, is the process under consideration. A base case design was developed, and process integration and intensification techniques were applied to reduce dependence on external utilities and to lower the overall capital investment. Waste heat recovery and off gas recycle were additional options used to intensify the overall energy consumption of the process. Emissions from the process were calculated from the EPA's guidelines. Economic and environmental metrics were then used to study the impact of integration and intensification techniques. Up to 70% reductions in CO2 emissions were achieved as a result of this approach to sustainable design. The Sustainability Weighted Return on Investment (SWROI) metric was evaluated for all cases. Multi-objective decision making for the optimum design was facilitated by the sustainability metrics augmented with the traditional economic criteria.

B. POSTER PRESENTERS

i) MORNING POSTER SESSION

1. Polymerized Ionic Liquid Triblock Terpolymers: Synthesis and Characterization

Patrick M. Lathrop and Yossef A. Elabd

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

Abstract:

Polymerized ionic liquid (PIL) block copolymers are a distinct set of block copolymers that incorporate the unique physiochemical properties of PILs (*e.g.*, high solid-state ionic conductivity, high chemical, thermal and electrochemical stability, and widely tunable physical properties) into block copolymer architecture, which allows for self-assembly into a range of nanostructures, where morphology type and domain size are tunable. To date, PIL block copolymers have been synthesized by a number of research groups and have shown distinct conductivity-morphology relationships as it relates to various applications. Several block chemistries have been explored, yet almost all reports are exclusive to (AB) diblock copolymers. Although AB diblock copolymers can provide orthogonal properties of high ion conduction and high mechanical strength in a solid-state material, there are limitations to AB diblock copolymers, such as limited set of morphologies, domain sizes, and a lack of means to achieve a combination of more than two properties simultaneously (*e.g.*, conductivity, strength, flexibility). Moreover, spatially connected 3D network morphologies, which often result in the highest ion conductivities, occur only over a small compositional range in AB diblock copolymers.

In this study, a PIL (ABC) triblock terpolymer was synthesized to explore a PIL-containing polymer with a richer compliment of properties, a wider diversity of cation/backbone chemistries, and a broader compositional range to obtain a variety of continuous 3D network morphologies. Specifically, poly(MMA-*b*-MEBIm-Br-*b*-HMA) was synthesized *via* sequential reversible addition-fragmentation chain-transfer (RAFT) polymerization and subsequently quaternized, where A block = methyl methacrylate (MMA), B block or PIL block = 1-[(2-methacryloyloxy)ethyl]-3-butylimidazolium bromide] (MEBIm-Br), and C block = hexyl methacrylate (HMA). Reaction kinetics of this PIL ABC triblock terpolymer were investigated and these results were utilized in scaling up the polymerization reaction to > 2 g quantities with narrow polydispersities and controllable block compositions. Chemical, thermal, morphological, and ion conductive properties were characterized using ^{1}H nuclear magnetic resonance (NMR) spectroscopy, elemental analysis (EA), gel permeation chromatography (GPC), differential scanning calorimetry (DSC), dynamic mechanical analysis (DMA), small angle X-ray scattering (SAXS), transmission electron microscopy (TEM), and electrical impedance spectroscopy (EIS).

2. Aramid Nanofiber/Functionalized Graphene Composite Electrodes for Structural Energy and Power

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Abstract:

Flexible, structural or even wearable electronics have recently become a significant and inseparable part of our everyday life. This has led to an urgent need for structural energy storage systems, such as structural batteries and supercapacitors. Therefore, the development of structural electrodes, electrodes that can simultaneously bear mechanical loads while storing energy, is crucial for the design of next generation electronics. Here, we report on multifunctional electrodes for supercapacitors, consisting of functionalized graphene oxide (f-GO) and aramid nanofibers (ANFs) fabricated through vacuum filtration. Graphene has remarkable properties such as high theoretical electrical conductivity, high surface area and excellent mechanical properties. On the other hand, recently developed aramid nanofibers, nanoscale Kevlar® fibers, are of great interest due to their exceptional mechanical properties, such as ultimate strength and stiffness. Functionalized graphene and ANFs were combined to create mechanically strong supercapacitor electrodes, where ANFs interact with f-GO through extensive hydrogen bonding and pi-pi interactions. The electrodes were characterized through scanning electron microscopy (SEM), Raman, and X-ray photoelectron

spectroscopy (XPS). The effect of the addition of ANF, as well as, of the functionalization of the GO sheets with different functional groups (-COOH and -NH2) on the mechanical and electrochemical properties, was examined. Tensile testing, cyclic voltammetry and galvanostatic charge-discharge tests were conducted to evaluate the mechanical and electrochemical performance of the fabricated structural ectrodes.

3. Radio Frequency Curing of Preceramic Polymers Loaded with Nano-fillers to Silicon Carbide Preforms

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Abstract:

Silicon carbide (SiC) structures are deployed to meet a wide range of defense and aerospace applications. These materials are often prepared by sintering but may also be prepared by high-temperature curing of preceramic polymers like polycarbosilanes. The limitation of polymer routes is slower curing processes and non-uniform curing due to heat transfer gradients. In this method, we are using carbon nanotubes (CNTS) as RF susceptors and heating CNT-polycarbosilane mixtures using RF sources. This leads to rapid curing of the polymers. In order to keep the mechanical integrity of the sample, we propose deposition and curing of thin layers. This technique has a wide scale application in additive manufacturing of SiC and mold casting as well. RF thermal spectroscopy technique developed by our group was used to find resonant frequency. Study of curing behavior of polymer for varying CNT loading and power was done. The extent of curing was shown by TGA and SEM.

4. Approach to Retard Oxidation During Processing of Colloidal Ti_3C_2 MXenes

Touseef Habib[1], Smit Shah[1], Yexiao Chen[2], Wanmei Sun[1], Miladin Radovic[2], and Micah J. Green[1]

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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 shown to be promising in a wide range of applications such as batteries, supercapacitors, electromagnetic shielding, and water desalination. However, Ti_3C_2 MXenes are prone to oxidation, which causes them to chemically degrade to TiO_2 over time and become impractical for desired applications. This makes processing of Ti_3C_2 MXenes difficult. In this study, we investigated oxidation of Ti_3C_2 MXenes in air, liquid media, and solid media. We characterized oxidation by monitoring TiO_2 content and conductivity of the processed films. We show Ti_3C_2 MXenes in solid media oxidize at lower rates relative to other media.

5. Ab-Initio Investigation of Dimethyl Disulfide as an Additive for Lithium-Sulfur Batteries

Ethan P. Kamphaus and Perla B. Balbuena

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Abstract:

Energy storage technology is an important field of study with strong economic and environmental driving forces. Batteries are ubiquitous and critical for much of modern technology like cell phones and electric vehicles. The current leader in rechargeable battery technology is the lithium ion (Li) battery. However, the Li battery is close to the theoretical limit of its energy storage but our technology requires more capacity. One promising battery system is the Lithium-Sulfur (LiS) battery which can surpass the Li battery by about 3 times the energy density.

Unfortunately, the LiS battery faces several challenging problems before it can be utilized commercially. One problems is known as the polysulfide shuttle reaction. This reaction is the consequence of the solubility of reaction products in the electrolyte. The polysulfide shuttle causes active material loss from the cathode and passivates both electrodes. Donghai Wang's group at Penn State University recently published a new strategy to counteract this effect: use a different electrolyte. Their new electrolyte

consisted of 50% DME and 50% dimethyl disulfide (DMDS) which showed increased battery performance. Wang et. al's experiment postulated several potential reasons for why they saw increased performance but were not able to determine exactly why.

We used density functional theory (DFT) to explore the theory and fundamentals behind DMDS's effect on battery performance to complement Wang et al's experimental work. Computational chemistry calculations were completed with Gaussian to determine reaction thermodynamics on the new reaction pathway that DMDS forms with the traditional sulfur reduction. We also investigated the passivation of the electrodes with the DMDS modified reduction pathway by solid state calculations with VASP. Electronic structure of the final reduction products that precipitate on the cathode were determined including DOS and other charge carrier calculations.

6. Ferrocene-Based Redox Switches for Reversible Single-Molecule Magnet Behavior in Dysprosium(III) and Erbium(III) Bis-Diamidoferrocene Complexes

Courtney M. Dickie[1], Alexander L. Laughlin[2], Joshua D. Wofford[1], Nattamai S. Bhuvanesh[1], and Michael Nippe[1]

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Abstract:

Single-molecule magnets (SMMs) are considered feasible candidates for next-generation high density data storage applications. SMMs featuring switchability of their magnetization dynamics are particularly attractive with respect to use in devices. This poster presentation will show that transition metal-based redox events may be used to influence slow magnetic relaxation at nearby anisotropic lanthanide(III) ions. The anionic homoleptic bis-diamidoferrocene complexes of Dy^{3+} (oblate) and Er^{3+} (prolate) may be reversibly oxidized by one electron to form the neutral species. The Dy^{3+} system can function as either an "on"/"off" or a "slow"/"fast" switch in the absence or presence of an applied dc field respectively, whereas the Er^{3+} system functions as an "on"/"off" switch in the presence of an applied dc field. Furthermore, results from ^{57}Fe Mössbauer spectroscopy, cyclic voltammetry and UV-Vis-NIR spectroscopy indicate the presence of significant electronic communication between Fe ions in the mixed valent compounds.

7. Systematic Process Intensification using Building Blocks

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

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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. 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.

8. A Novel Derivative-Free Optimization Method on Single Dimension Projection

Ishan Bajaj and M. M. Faruque Hasan

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Abstract:

With the advent of high-fidelity, complex process modeling and simulation in many areas including computational fluid dynamics-based reactor design, Nonlinear Algebraic and Partial Differential Equations (NAPDE)-based multiscale optimization, data-driven methods are gaining more importance than ever. Most often, these optimization problems are formulated as black-box problems where the objective function and/or constraints cannot be expressed analytically as explicit functions of decision variables. This implies that the values of the objective and/or constraints become available only after performing a full-scale expensive simulation. To this end, derivative free optimization (DFO) has emerged as a promising approach to optimize black-box problems.

In this work, we present an algorithm to address multi-dimensional black-box problems based on projection onto a one-dimensional space. Specifically, we consider a problem of minimizing $G(t)$, which can be interpreted as the projection of the original objective function $f(x_i)$, $i = 1, \ldots, n$ taken in the t-space such that i=1nxi=t. We show that the minimum of $G(t)$ also corresponds to the minimum of $f(\mathbf{x})$. This enables us to solve the original optimization problem in two steps. The first step involves identifying $G(t)$ and is referred as the inner loop. In this work, the inner loop is applied at discrete values of t (t1, t2, …,tk). Once the solution at the previous t (tk-1) is known, sensitivity theorem is utilized to obtain close solution for the inner loop at next t(tk). The second step is optimizing the univariate function $G(t)$ to find the solution of the original problem. The algorithm is applied to a large set of test problems and compared to existing model-based DFO solvers.

9. Modeling, Simulation and Optimization of Hybrid Adsorption-Reaction Systems

Akhil Arora, Ishan Bajaj, Shachit S. Iyer, and M. M. Faruque Hasan

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Abstract:

Intensified adsorption-reaction processes have shown promise for obtaining higher reaction conversions, and better process efficiency and integration in equilibrium-limited reactions. In these processes, in-situ removal of the reaction byproducts from the gas phase reaction mixture, by a solid adsorbent, favors further production of non-adsorbed product. Hydrogen has been produced via sorption-enhanced steam methane reforming (SE-SMR) and sorption-enhanced water gas shift (SE-WGS); these intensified reactions have shown significant reduction in temperature, and higher hydrogen product purity and limiting reactant conversions in comparison to the conventional reactions. Therefore, the practical utility for efficient designing of reactor-adsorber systems using high-fidelity mathematical models is indispensable. However, the dynamic nature of such processes, and the complex and coupled multiphysics nature of the systems make their modeling and simulation a complicated task.

In this work, we have developed a high-fidelity generalized reaction-adsorption modeling and simulation (GRAMS) framework. For demonstrating the capabilities of GRAMS, the simulations are performed for several configurations of the column containing (i) pure catalyst, (ii) pure adsorbent, (iii) heterogeneously-compartmentalized adsorbent and catalyst, and (iv) homogeneously-distributed uniform mixture of adsorbent and catalyst. The model predictions show excellent agreement with experimental observations for SE-SMR, SE-WGSR, conventional SMR and pressure swing adsorption. GRAMS is then coupled with in-house black-box optimization solvers for simultaneous identification of optimal sequence and types of process steps, and optimal process operating conditions including pressure, temperature, steps duration, feed composition and flow rate, and adsorbent-to-catalyst ratio.

10. Toward a Systematic Framework for the Synthesis of Safely Operable Process Intensification Systems

Yuhe Tian[1], M. Sam Mannan[1,2], and Efstratios N. Pistikopoulos[2,3]

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Abstract:

Modular process intensification offers the promise to involve multifunctional phenomena at different time and spatial scales to efficiently overcome process limitations and maximize synergy effects. However, this highly integrated scheme often reduces the degrees of freedom for safe operation and process control, thus arousing concerns from process safety and operability perspective. Despite increasing efforts in recent publications towards a systematic strategy to deliver intensified processes, there is a lack of approach to simultaneously synthesize intensified but safely operable systems. To address this challenge, we will present an integrated framework, which embeds inherent safety, flexibility, and controllability analysis in a phenomenological representation framework to derive intensified designs with guaranteed safety and operability performance.

The proposed framework features (i) superstructure-based process synthesis using Generalized Modular Representation Framework to give the resulting design configurations, where multifunctional mass/heat exchange modules are employed as building blocks; (ii) high-fidelity dynamic modeling and simulation; (iii) operability analysis, comprising flexibility analysis for accommodation of uncertainty, risk assessment for inherent safety evaluation, together with controller design in multi-parametric model-based predictive control (mp-MPC) scheme following the PAROC framework; and (iv) in-silico closed-loop validation to bridge between steady-state synthesis and dynamic modeling and to ensure targeted performance during both operation modes. As the first step of a broader scope of process intensification systems, we apply the proposed framework to a case study on heat exchanger network (HEN) synthesis, which opens up the potential for thermal process intensification, as well as can be expanded to mass/heat exchanger network synthesis. The results indicate that significant improvements in HEN design configurations can be obtained to enhance safety and operability.

11. Effect of Carbon Dioxide-Sustained Adsorption using Ion-Exchange Resin on Mixed-Acid Fermentation

Haoran Wu, Samarpita Roy, Kefan Yang, and Mark Holtzapple

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Abstract:

The carboxylate platform is a biomass-to-energy process that converts biomass into hydrocarbon fuels or chemicals. Using mixed-cultures of microorganisms, five mixed-acid fermentation systems were established. Carbon dioxide-sustained resin adsorption column was designed and the effects of carbon dioxide flowrate in carboxylic acids uptake capacity were measured. Different amount of weak base anion-exchange resin (Amberlite IRA-67) were employed to adsorb the carboxylic acids produced from the established fermentation systems in the presence of carbon dioxide. The conversion, yield and selectivity with or without adsorption in each system were calculated and compared.

12. Fire Incidents in Offshore Oil and Gas Rigs: Analyses of Incident Investigation Reports

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Abstract:

In order to learn from past incidents and prevent future disasters from occurring, it is important to identify underlying factors that led to the incidents. Fire incidents are rather common on offshore oil and gas facilities. In an attempt to identify the common causes behind such incidents, the current work focuses on analyzing 137 investigation reports on fires that occurred on offshore oil and gas facilities located in the Gulf of Mexico, made available by Bureau of Safety and Environmental Enforcement (BSEE). These reports have been analyzed using a systematic methodology to generate statistical data on leading causes and lagging measures

arising from various technical, operational, human and organizational issues that contributed to the incidents. Initially, the investigation reports had categorized the findings into 9 direct causes (equipment failure, human error, external damage, slip/trip/fall, weather related, leak, upset H20 treating, overboard drilling fluid and other), of which equipment failure and human error were found to be the most common ones. However, our analysis of the narrative parts of the reports found that apart from the 9 broad causes, there were many other factors that contributed to these causes. The most recurring contributing factors were job safety analysis, procedure (including procedural deviation and improper procedure) and maintenance related issues. Others such as improper supervision, improper communication, design flaw etc. were also identified. This work thus provided a deeper insight about the issues that led to the past incidents and helped identify the areas of concern that needs improvement to achieve process safety excellence in offshore facilities to prevent future disasters from recurring.

13. Calorimetry Studies of Benzoyl Peroxide

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Abstract:

Organic Peroxides (OP) are widely used in petrochemical industry as initiators. Their unstable O-O bonds make them very useful, but also hazardous due to highly exothermic nature of decomposition, which can result in runaway reactions. Benzoyl peroxide (BPO) is one of the most commonly used OPs in industry and the hazards associated with its processing, storage and transport are revealed in many incidents. Benzoyl peroxide can decompose under favorable conditions and release large amounts of energy in short time. The decomposition reaction can ultimately lead to runaway reaction, posing great hazard of high temperature and high pressure. The most critical control factors of thermal decomposition and possible explosion of benzoyl peroxide are temperature, structure, and impurities or extraneous matter. This research is a comprehensive study of the runaway behavior of BPO hybrid system using isothermal and adiabatic calorimeters. The aim is the advancement of understanding the thermal decomposition of BPO under various conditions from both experimental and theoretical aspects. More specifically, this research will systematically study and develop thermodynamic and kinetic parameters related to decomposition of BPO, and further the use of this particular knowledge to mitigate the risks in storage, transportation and manufacturing process.

14. Safety Assessment of Secondary Alcohol Oxidation with Hydrogen Peroxide

Yue Sun[1], Lei Ni[2], Maria Papadaki[3], Wen Zhu[1], Juncheng Jiang[2], and M. Sam Mannan[1]

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Abstract:

Ketones are produced on massive scale in industry as solvents, polymer precursors, and pharmaceuticals. Current ways of producing ketone through alcohol dehydrogenation are energy intensive and usually expensive, hazardous and toxic due to employing strong oxidizing agents. In 1997, Kazuhiko Sato, et al., found a way of producing ketones via 30 % hydrogen peroxide oxidation of alcohol, and tungstate as catalyst along with a phase transfer catalyst. This method is considered as 'green chemistry' since it is organic solvent- and halide-free. Lots work has been done later focusing on different catalysts and experimental conditions as well as their effects on yields of different ketones in laboratory.

However, there are safety concerns for scale-up regarding this reaction system because of its runaway potentials. Thus, the purpose of this project is to conduct a comprehensive study of thermal and kinetic behavior of this reaction system. Calorimeters, such as DSC and Phi-Tec, are used to help study, experimentally and theoretically, these reactions under normal operating and runaway conditions. Here, we report the thermal hazard assessment of these reactions and discuss the DSC results as well as GC/MS analysis of chemicals that produced through the test. The findings will be further used to propose measures for safer design and scale-up of this reaction process with runaway potentials.

15. Studying The Effects of Obstacle Configuration and Fire Suppressants on Flame Propagation Regimes

Cassio B. Ahumada[1], Eric Petersen[2], and M. Sam Mannan[1]

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Abstract:

In respect of vapor cloud explosions, there are two main combustion modes: deflagration and detonation. Deflagrations occur when the flame front travels at subsonic speeds leading to overpressures with the same order of magnitude as the atmospheric pressure. Unlike deflagrations, detonations are characterized by supersonic flame propagation velocities and significant overpressures. Several experimental studies have shown that, when the proper conditions are met, the flame front may accelerate reaching the detonation combustion mode; a phenomenon known as deflagration-to-detonation transition (DDT). However, more recent large-scale tests have demonstrated that intermediate states between laminar deflagrations and CJ detonations are more likely to happen for fuels with low and medium reactivity, such as methane and propane. Therefore, this research project focus on studying experimentally and numerically intermediate combustion regimes during deflagration-to-detonation transition. The ultimate goal is to understand the effects of layout and fire suppressants on the final flame speed.

16. Predicting the Stability of Pt^{II}-Based Molecular Gyroscope Isomers

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Abstract:

Recent efforts to synthesize molecular gyroscopes containing a platinum core have unveiled several competing molecular architectures (see abstract graphics, compounds a-d). We sought to understand if there exists any thermodynamic preference for one of these species, but moreover, to probe how the linker length (n) and ligand set (L = F, Cl, Br, I, H, Me, Ph) would impact the relative stability of a-d as this could help us steer the experimental endeavors in a clear direction. Density functional theory was used to probe these issues using both gas-phase calculations and solvent corrected models. Dispersion corrections were also implemented to account for the dispersion interactions that were of particular importance for compounds with large linker length (n = 18, 20, 22). Calculation data were compared to experimentally harnessed X-ray structures, which showed good structural agreements. It was concluded that for short-medium linker lengths (n = 10, 12, 14), the gyroscope architecture (a) proved to be the most stable isomer in the presence of small to medium sized ligands (L = H, F, Cl, Br, I). However, the "parachute" structure (b) was favored for larger ligands (L = Me, Ph) with short linker lengths. The "ear-type" structures (c, d) were high in energy relative to a-b with short linker length species (n = 10-14) due to steric effects exerted in two of the smaller macrocycles, or "ears". Interestingly, c and d are closer in energy to a when the linker length increases ($n \geq 16$), and this tendency have also been experimentally observed. These investigations will help us to direct the synthesis to specifically target a-d by providing a rationale for the stereoelectronic underpinnings on how components such as ligand type and linkage length impact the relative stabilities.

17. Study on the Interfacial Interaction between Carbon Nanotubes and Catalyst, and the Effect in Tube Diameter

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Abstract:

Single-walled carbon nanotubes (SWCNTs) are seamless cylinders of graphene that have been at the forefront of nanotechnology research for the past two decades. They possess a range of exceptional properties including high strength (~37 GPa), thermal conductivity (~3500 W/m/K) and ballistic electronic transport. Importantly, they can have semiconducting, semi-metallic, or metallic conductivity depending on their chiral angle (χ), i.e. the angle between the tube axis and the edge of the graphene lattice. While mass-produced SWCNT powders are adequate for some applications, many emerging applications require stricter control over SWCNT properties and architectures, necessitating targeted growth, i.e. tailoring the physical properties of the SWCNTs (diameter, orientation/architecture, etc.) during synthesis to match the requirements of a particular application.

This project attempts to prove the key role of the catalyst – graphene interaction in the chirality selectivity of carbon nanotubes (CNT) and therefore, the intrinsic relation between catalyst size and nanotube diameter. We work on the assumption that the curvature energy is one of the most influential factors in the nanotube's formation reaction and a decisive step to determine the diameter of the nanotube during the growth. The calculation of interlayer binding energies using density functional theory (DFT) and pseudopotential functions has been valuable to find the transition diameter between fullerene and tube. Also, we propose a new relation that links theory to measurable thermodynamic properties such the surface tension, and surface energy. This is just the first step to bring light to the yet undiscovered reigning principle in the nanotube's diameter stability during nucleation.

ii) AFTERNOON POSTER SESSION

18. Electrochemical Investigations of Electroactive Redox Polymer for use in Energy Storage Devices

Kasturi Sarang[1], Hysoung An[1], Andrea Miranda[3], Jodie L. Lutkenhaus[1,2], and Rafael Verduzco[3,4]

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Abstract:

Future is dependent on electrochemical energy storage (EES) systems which will have a tremendous role in technical applications like computers, communication devices, electric vehicles, laboratory equipment etc. Fossils fuels are depleting, and we can already see the world moving towards EES systems. Polymers have a prominent place in EES, not just as an electrolyte, but also in solid state batteries, especially electrodes. Recent focus is on organic polymers since they are sustainable, nontoxic and its possible to fabricate lightweight flexible devices. This study introduces an organic pi-conjugated redox active polymer, poly(fluorene-alt-napthalene diimide) (PFNDI), which can be a potential n-type polymer in EES systems. N-type polymers have shown to lack electrochemical stability and have very high impedance, thus making them unsuitable for fast charge/discharge kinetics. However, we have shown that PFNDI can be stably and reversibly doped with high ion and electron conductivity, thus enabling realization of fast rechargeable batteries. PFNDI has a redox active unit which assist in doping process and a pi-conjugated unit which assists in electron and ion transfer. Energy is storage via exchange of dopants and electrons during charge/discharge. We have done a detail fundamental study of energy storage in n-type polymer. We evaluated this polymer as a charge storage material for rechargeable Li batteries and it delivers 92% of its theoretical capacity at very high rate of 1000C. This study introduces a new organic polymer which has a potential application in all polymer flexible battery and/or capacitor.

19. Saturated N-heterocyclic Cationic Polymers: Synthesis and Stability

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Abstract:

Polymers containing unsaturated N-heterocyclic cations (i.e., imidazolium) have been synthesized and investigated for various applications, including alkaline fuel cells and batteries. Recently, results have shown higher alkaline chemical stability for polymers bearing a saturated N-heterocyclic cation (pyrrolidinium) versus an unsaturated imidazolium cation. Additionally, several studies on small molecules have reported increasing stability with increasing saturated N-heterocyclic cation size and this was attributed to decreasing ring strain with increasing cation size. However, to date, few studies have systematically investigated polymers containing saturated N-heterocyclic cations, specifically N-heterocyclic cations with larger ring sizes (i.e., azepanium, azocanium, azonanium). In this study, styrene-based saturated N-heterocyclic cationic (SNHC) polymers with various covalent attached cations (methylpyrrolidinium, methylpiperidinium, methylazepanium) were successfully synthesized to investigate the influence of ring size/strain on the properties of SNHC polymers. Functionalization of poly(vinylbenzyl chloride) was employed to covalently attach cations onto polymer backbone, followed by anion exchange metathesis, resulting in polymers with bromide counter anions. Alkaline chemical stability, temperature and humidity dependent water uptake, and ion conductivity of these SNHC polymers were measured and will be reported in regards to the relationship with ring size/strain. This work provides a fundamental understanding of the ring size/strain effect in SNHC polymers and further introduces a promising chemistry for producing highly stable and ion conductive solid-state separators for alkaline fuel cells and batteries.

20. High-Resolution Scalable Propylene/Propane Separation for ZIF-8 Polycrystalline Membranes on Ceramic Tubular Support

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Abstract:

Zeolite-imidazole frameworks (ZIFs) have been extensively studied as a new membrane material for gas separations due to their robust synthesis protocols, chemical and thermal stability, and well-defined ultra-micropores (~ 2 to 5 Å).1, 2 ZIFs are comprised of metal centers (Zn, Co, and Cd) and bridging imidazole-based ligands. ZIF-8, composed of zinc nodes and 2-methylimidazole linkers, has been shown very promising for propylene/propane separations since its effective aperture size lies in between propylene (~ 4 Å) and propane (~ 4.2 Å).3 In fact, some of the polycrystalline ZIF-8 membranes synthesized by various methods have been reported to exhibit impressive propylene/propane separation factors up to 200.4, 5These highly propylene-selective ZIF-8 membranes were supported mostly on alumina disks or occasionally on hollow fibers (polymer or ceramic).

For their large-scale industrial applications, however, the productivities of ZIF-8 membranes must be significantly improved. One way to increase the membrane productivity is to increase membrane area per volume. As such, current disk supports are not desirable. Though hollow fiber supports (either polymer or ceramic) are most desirable, they are unlikely to be used for large-scale applications in near future. This is because ceramic hollow fibers are highly fragile while polymer hollow fibers require much more development. While hollow fiber supports are transformative, ceramic tubular supports are readily available for large-scale applications. For example, ceramic tubular supports have been used for commercial polycrystalline zeolite membranes.7 Though ZIF-8 membranes on ceramic tubular supports were reported, none of those membranes showed promising propylene/propane separation capabilities.

Here, we would like to present polycrystalline ZIF-8 membrane supported on alumina tubes showing high propylene/propane separation performances. The tubular membranes were synthesized using our microwave seeding and secondary growth method. The effects of the synthesis parameters on the microstructures of tubular ZIF-8 membranes will be presented. Finally, the propylene/propane separation performances of ZIF-8 membranes supported on alumina tubes will be discussed.

21. Application of Electrochemical Impedance Spectroscopy for The Study of Degradation Behavior of Nanowire Thin Films in Simulated Industrial Environments

Pranav Kannan[1,2], M Sam Mannan[1,2], and S. Vaddiraju[1,2]

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Abstract:

Silicon (Si) and Copper (II) Oxide (CuO) Nanowires (NWs) are substrates which offer the possibility for diverse applications in battery anodes, gas-sensing, PV modules, etc. due to their ease of surface modification, large surface area to volume ratio and scalable production. An important limitation is the lack of understanding of fouling and degradation processes in aggressive field environments such as those faced in the oil and gas industry. To improve the understanding of the electrochemical processes, two environments, 3.5% NaCl and simulated produced water (brine solution) were utilized in a three-electrode configuration with a high-internal resistance potentiostat to generate impedance spectra over a 24-hour period. The Nyquist plots indicated the presence of diffusion limitations at low frequencies for the silicon nanowires, and at high frequency there were contributions from external connections and ionic conductions to exhibit pure resistive behavior. The intermediate frequencies exhibited the individual contributions from the nanowire elements to the surface resistance. The Nyquist plots for the copper oxide nanowires indicated the increase in the surface resistance with time, which is attributable to the formation of passive film due to hydroxide formation. In contrast, the silane hydrolysis can be attributed to the decrease in surface resistance with time for the silicon nanowires. The equivalent circuit models for both the systems are utilized for further explanation of the surface processes.

22. Cone Calorimeter Analysis of Flame Retardant Poly(Styrene) Nanocomposite

Lubna Ahmed[2], Bin Zhang[2], Ruiqing Shen[3], Zhengdong Cheng[1], Qingsheng Wang[3], and M. Sam Mannan[1,2]

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Abstract:

The widespread application of polymers in the domestic and industrial life of people necessitates the study of its flammability. Polymer, being hydrocarbon, is a source of fuel in any fire scenarios. Flame retardant nanofiller can be one potential barrier to deteriorate the flame spread at the event of a fire. In the present study, silica and montmorillonite nanofillers will be embedded via *in-situ* method within the polystyrene matrix for forming fire retardant polymer nanocomposite. Polymer-nanocomposites 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 of nanocomposites and analyze the reaction of the same to the fire, cone calorimeter has been used. Both neat polystyrene and polystyrene nanocomposites have shown the trend of a thermally thick charring polymer in the heat release rate over time data. The nanocomposites had an overall better flame retardancy than the neat polystyrene in terms of lower peak heat release rate, lower average mass loss rate and enhanced char formation. The nanocomposites had also reduced smoke emission with lower CO and CO_2 yield compared to the neat polystyrene. The overall flame retardancy was enhanced as the nanofiller loading was increased for both the nanosilica and MMT nanocomposites.

23. Combined High Stretchability and Gas Barrier in Hydrogen-Bonded Multilayer Nanobrick Wall Thin Films

Shuang Qin, Yixuan Song, Michael E. Floto, and Jaime C. Grunlan

Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843

Abstract:

Stretchable gas barrier coatings, that can maintain their barrier performance when subjected to high strain, are highly desired for flexible electronics protection, pressurized systems (e.g. tires and gas seals) and various types of food and pharmaceutical packaging. In this study, we demonstrate a stretchable high oxygen gas barrier nanocoating prepared with water-soluble and environmentally benign materials using layer-by-layer assembly. Polyethylene oxide (PEO) was alternately deposited from water with an aqueous mixture of polyacrylic acid (PAA) and montmorillonite (MMT) clay. The oxygen impermeable MMT platelets were highly exfoliated and aligned within the PEO/PAA polymer matrix. Ten bilayers of this multilayer nanocoating, with a thickness of 432 nm, improves the oxygen barrier of a 1mm polyurethane rubber by more than 50X after exposure to a 20% strain. This system, which provides the best stretchable oxygen barrier to-date in the open literature, shows great potential for use in a number of everyday products.

24. Advancing the Production of Olefins and Aromatics from Natural Gas Via Methanol: Chemical Looping for Syngas Generation

William W. Tso[1,2], C. Doga Demirhan[1,2], Alexander M. Niziolek[3], Onur Onel[3], Christodoulos A. Floudas[†], and Efstratios N. Pistikopoulos[1,2]

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Abstract:

Due to technological advances in the shale gas industry, the supply of natural gas in the United States has greatly increased (37% since 2008) and its price has significantly dropped ($2.52/MMBtu in 2016). The shale gas boom has not only revitalized the U.S. economy, but also rejuvenated interests in C1 catalysis toward the production of chemicals typically derived from petroleum

refining. Olefins (ethylene, propylene, butane isomers, butadiene) and aromatics (benzene, toluene, xylenes) are examples of valuable chemicals in high demand.

A judicious utilization of natural gas resources necessitates a systematic analysis of all available processing routes. To this aim, a gas to olefins and aromatics (GTOA) superstructure has been developed and includes several olefins and aromatics production technologies. Previous works investigated reforming as the primary method to convert natural gas to syngas and demonstrated the profitability of GTOA processes. Recently, the benefits of chemical looping for syngas generation have been observed in lowering the breakeven oil prices for a gas to liquids (GTL) process. In this work, we incorporate chemical looping into the GTOA superstructure as an alternative to reforming and study its impact on chemicals production.

Process synthesis of the GTOA superstructure forms a large-scale nonconvex mixed-integer nonlinear model (MINLP). A tailored deterministic global optimization branch-and-bound algorithm is used to solve the MINLP and determine optimal natural gas refineries with the highest profit. Several case studies are investigated to compare chemical looping against reforming for natural gas conversion. The effect of different plant capacities and product ratios are explored as well. Key topological selection of process technologies will be discussed.

25. Fault Detection and Diagnosis of Continuous Processes via Non-linear Support Vector Machine Based Feature Selection

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Abstract:

Advances in sensor and data collection technologies has valorized data-driven modeling approaches in process monitoring and fault detection in process systems engineering. Today, machine learning and pattern recognition techniques play a significant role in attaining actionable insights and decision-making from the vast amounts of available process data by building accurate and robust data-driven models. One of the most popular machine learning techniques is Support Vector Machines (SVMs) which allows the use of high dimensional feature sets for learning problems such as classification and regression. Yet reducing the dimensionality of the feature space in data-driven modeling, known as dimensionality reduction and feature selection, is still a key task in improving model accuracy as well as decreasing *a priori* data collection, which in turn yields enhanced efficiency in chemical processes.

In this work, we present the application of a novel non-linear (kernel-dependent) SVM-based feature selection algorithm to process monitoring and fault detection of continuous processes. The developed methodology is derived from sensitivity analysis of the dual SVM objective and utilizes existing and novel greedy algorithms to rank features that also guides fault diagnosis. Here, we train two-class SVM models to detect known faults where the manipulated and measured variables of the process constitute the input feature space, and instances of normal and faulty operation yield training samples for our SVM models. The feature selection algorithm is used to improve the accuracy of fault detection models and perform fault diagnosis. We present results for the Tennessee Eastman process as a case study and compare our approach to existing approaches for fault detection and diagnosis.

26. Multi-scale Optimization of a Novel Separation and Storage Technology for Natural Gas

Shachit S. Iyer, Salih E. Demirel, and M. M. Faruque Hasan

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

Abstract:

Significant efforts have been undertaken in the past for the separation, storage and transportation of methane from sources such as natural gas, shale gas, landfill gas and biogas which can often have high impurity content. Existing adsorption-based separation processes involve multiple pressure changes at different steps and multiple individual units resulting in additional cost. We propose a novel combined separation and storage (CSS) technology to simultaneously separate and store methane in a single column while

eliminating separate steps [1]. However, the following challenges remain: (i) materials and technologies with high selectivity for methane separation often do not have high capacity for storage, and (ii) materials and technologies with high capacity for methane storage often do not have high selectivity for separation. For application in the CSS process, the adsorbent material should simultaneously possess both high methane selectivity and storage. Design of such a technology requires a rigorous multi-scale modeling and optimization approach. The adsorption of gases in the column is described using a non-linear algebraic partial differential equation model which is discretized over space and time domains to formulate and solve an optimization problem. The optimal operating conditions and adsorbents which would maximize storage of methane while maintaining a desired level of purity can then be obtained. Solutions from simulations are provided as warm starts to the optimization algorithm to aid in convergence.

27. Multi-objective Stochastic Optimization for Preventive Maintenance Planning in Chemical Plants

Christopher Gordon, Monir Ahammad, 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

Abstract:

Maintenance planning and process operations in chemical manufacturing facilities are subject to several sources of uncertainty ranging from volatile feedstock prices to uncertainty in the level of demand. In the context of assuring the integrity of assets in ageing chemical plants, the present research focuses on uncertainty in equipment availability and develops a novel multi-objective stochastic mixed-integer nonlinear optimization algorithm for preventive maintenance planning. The algorithm factors in uncertainty to arrive at robust optimal solutions in contrast with other approaches such as risk-based inspection and deterministic optimization. In addition, it simultaneously considers the two competing objectives of cost minimization and system availability maximization to decide on the optimal maintenance frequency, set of online equipment and process flowrates at each time stage.

The proposed approach consists of two main steps. In the first step, the system is represented as a dynamic Bayesian network to capture complex interactions between system components, identify critical failure pathways, and characterize the overall risk of system failure. In the second step, the multistage stochastic optimization subproblem is formulated over a shrinking time horizon to progressively incorporate decisions and information from prior time stages into the decision-making process. Following system representation and problem formulation, the overall multi-objective optimization problem is solved using the epsilon-constrained method to obtain the optimal maintenance policy. The overall optimization problem is non-convex and large-scale and computational difficulties are tackled within the algorithm using structure-based decomposition strategies such as Generalized Benders decomposition, or via metaheuristic optimization techniques such as simulated annealing.

The results of the research include: (i) obtaining a robust optimal expected preventive maintenance plan and operating schedule, and (ii) provision of a Pareto front of optimal solutions from which the decision maker can select. This robust approach combining the techniques of Bayesian network-based risk assessment and nonlinear stochastic programming is illustrated with a case study and can be used to improve overall equipment availability and maximize plant productivity.

28. Identify Weak Signals using Data Mining Techniques

Mengxi Yu, Noor Quddus, 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

Abstract:

Despite accumulated process safety knowledge and analysis tools of safety management, catastrophic incidents in process industries still occur. Most incidents are led by an incubation period when a chain of discrepant events develops and accumulates unnoticed. Some weak signals are only recognized after incident investigations, but are difficult to be recognized and interpreted before the incidents occur. On the other hand, a large volume of different types of data exist in process industries, including process data, maintenance and inspection data, incident reporting data and so on. Thus, the study is aimed to learn from historical database in process industries by using data mining to identify weak signals and predict occurrence of unwanted events/incidents. In current phase of the study, data is generated by modeling and simulation to be analyzed by data mining. The study will be decomposed to few tasks: define weak signal, understand and analyze the human/ organizational/ technological functions involved in a methyl

methacrylic polymerization process, generate data for the involved functions and corresponding scenarios, and finally develop a predictive model using data mining techniques to identify weak signals.

29. Mapping Review of Reactive Chemicals Hazards Research

Hallie Graham 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

Abstract:

Reactive chemicals are a major hazard affecting both the processing, storage, and handling of chemicals, powders, and pharmaceuticals that can lead to serious consequences such as fires, explosions, and toxic gas releases. In the 2003 Chemical Safety Board's Reactive Hazard Investigation of 167 serious accidents over 40 classes of chemicals were identified with no one dominating class involved and most were not even listed as reactive chemicals. This mapping review takes a systematic approach to review the study of reactive chemicals. A comprehensive look at the field of reactive chemical comparing the types of chemical, equipment, and computational techniques used to understand and handle their highly volatile nature. The review shows the most common types of reactive chemical studied in literature. The comparison of the laboratory equipment such as calorimeters used and the computational techniques available. Mapping the use of the different techniques within different classes of reactive chemicals to identify gaps.

30. Developing Probabilistic Barrier Failure Models to Predict Kicks while Drilling

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

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

[2]Harold Vance Department of Petroleum Engineering, Texas A&M University, College Station, TX 77843

Abstract:

Predicting a kick timely and efficiently is often a challenging task due to the complexities of drilling and other well intervention activities. Leading indicators based probabilistic barrier failure models for different stages of drilling are developed in this work to assess performance of primary well control barrier – hydrostatic head. These models would help to determine the probabilities of kick initiating events and identify key leading indicators for predicting kicks and preventing blowouts. The key causal factors for primary well control barrier (hydrostatic head) failure have been identified by conducting fault-tree analysis and analyzing historical incident data. Abnormal pore pressure and swabbing are found to be the major contributors for low hydrostatic head or mud column failure. To predict abnormal pore pressure and swabbing events effectively, leading indicators model are developed combining organizational, operational and real-time indicators. A Bayesian network tool is used to construct probabilistic well barrier failure models for these causal elements. The probability distribution for observing changes in real-time parameters when a kick is developing due to abnormal pore pressure or swabbing are also determined. These parameters are function of both kick initiating events and some influencing organizational factors. This study would allow both predictive (causes to effect) and diagnostic (effect to causes) reasoning of kicks and blowouts for better understanding of well control system while drilling. Developed risk models enable informed decision making with a relatively clear picture of the risk of barrier failure and provide useful information on actions required to prevent escalation of well control events.

31. Thermal Decomposition of Mono-Nitrated Toluene (MNT) with Additives

Wen Zhu and Chad V. Mashuga

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

Abstract:

On September 21st 1992, an explosion happened in Castleford, UK, at the distillation unit, owned by Hickson & Welch Ltd. The incident killed 5 people and caused nearly 200 injuries. The main reason is due to the decomposition of mono-nitrated toluene (MNT). Nitrated aromatic compounds present a potential run-away reaction threat to the chemical process industry, due to its unstable structure and extensive heat release during upset situations. This study employs the Advanced Reactive System Screening

Tool (ARSST) to study the effects of various common contaminants on MNT's thermal decomposition, including sodium nitrate, sodium hydroxide, and sodium carbonate. Experimental parameters and results such as 'onset' temperature, pressure increase rate, temperature increase rate and maximum temperature are present.

32. Optimization of Flame Retardants on Commercial Aircrafts

Mazdak Mina 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

Abstract:

To ensure the long-term health of pilots and flight attendants on planes, while also keeping planes safe, an optimization analysis, risk assessment, and root cause analysis literature review, with some lab work, on the flame retardant chemicals and additives used on planes needs to be done. Flame retardants are known carcinogens that are widely used on household and commercial materials to prevent the ignition and spread of fires in homes and businesses. Due to their carcinogenic design, overexposure to flame retardants over an extended period of time has also been shown to cause cancer, most recently involving long-term workers (pilots and flight attendants) on commercial planes. In order to balance the safety risk of a plane catching fire with the health risk for the workers on a plane, an optimization analysis needs be done to confirm the optimum level of flame retardant chemicals is needed to minimize both risks and save the most lives. In addition, both a risk assessment and a root cause analysis needs to be done to determine where the biggest risks lie, what the greatest causes of injury or health effects are, and where optimization would be most effective. Finally, some lab work can also be done to find less carcinogenic or non-carcinogenic flame retardants that may also be effective as a long term solution to this problem. Overall, by doing the previously mentioned literature review and analyses, a solution to the problem of balancing safety and risk involving flame retardants on planes can be found.

33. Formation of Multi-layer Graphene Nanosheets with Strong Sulfur-Carbon Interaction and Enhanced Sulfur Reduction Zones for Lithium-Sulfur Battery Cathodes

Saul Perez Beltran and Perla Balbuena

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

Abstract:

The Lithium-sulfur battery is one of the most promising alternatives to allow rechargeable batteries do the big leap of rechargeable batteries from portable consumer electronics to high demanding energy applications. Before commercial implementation, however, much work must be still done to make improvements concerning cycle-life, stability, and electrochemical activity. A common strategy to implement sulfur-based cathodes is using sulfur-carbon composite materials. These composite structures might help to solve one of the most common issues the Li/S batteries face, the insulating nature of sulfur and the formation of soluble lithium sulfide intermediates. Deeper understanding of the lithiation mechanisms of these composite cathodes is still needed.

In this work we present a novel sulfur/graphene architecture emulates the electrochemical behavior of the Li-S battery cathode, promoting the S-C interaction through the edges of graphene sheets. Structural stabilization and S reduction calculations are performed with classical reactive molecular dynamics and density functional theory. This methodology allowed us to account for the collective behavior of the S and graphene structures. The S encapsulation induces ring opening, and the S phase evolves into a distribution of small chain-like structures interacting with C through the graphene edges. The lithiation calculations showed the Li_2S phase grows around ensembles of parallel graphene sheets during S reduction. No diffusion of S or Li between graphene sheets are observed and extended Li_2S domains bridging the space between carbon ensembles are suppressed. The results emphasize the importance of morphology on the electrochemical performance of the composite material. The sulfur/graphene model outlined here provides new understanding of the graphene effects on the S reduction behavior and the role that van der Waals interactions may play in favoring S reduction reactions and enhanced polysulfide trapping.

34. Magnetically Driven Functionalized Nanoplatelets Pickering Emulsion for Removal of Oil Contaminants from Water

Dali Huang[2], Minxiang Zeng[2], Lecheng Zhang[2], Arun Sabapathy[2], Janet Sajan[2], and Zhengdong Cheng[1]

[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, College Station, TX 77843*

Abstract:

There is an immense need for efficient cleanup and recovery of industrial grade oil in today's society. Incidents like the BP Deepwater Horizon oil rig explosion in the Gulf of Mexico in 2010 and Sanchi tanker collision in East China Sea in Jan. 2018 have caused huge oil spill and tremendous harm to the environment. This has resulted in the loss of billions of dollars due to the loss of products and cleanup efforts, which now has drawn considerable attentions for the environmental merits. The purpose of our research is to develop an effective and inexpensive method to absorb crude oil from oil-water mixtures. Functional magnetic nanoplatelets can be designed as Pickering emulsion surfactant for targeting removal oil contaminants from seawater. After introducing magnetic nanoparticles into water-oil mixtures, small oil droplets will be stabilized by two-dimensional Pickering nanoemulsifier and can be easily controlled to move by the external magnetic field. The advantage of utilizing magnetic particles to extract oil droplets from mixture is that oil droplets can move as designed direction and easily be reclaimed for use. Small stable oil droplets are relatively hard to remove and costly, but adding magnetic nanoparticles and establishing an application with magnetic field can restore large amount of extracted oil with a high speed. This magnetic particle approach can be considered as an environmental and promising technology for oil water separation.

35. Microfluidic Microbiologically Influenced Corrosion (M-MIC) Models

Susmitha Purnima Kotu[1], Sam Mannan[1] and Arul Jayaraman[1]

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

Abstract:

Several industries such as oil and gas, chemical, marine and aviation industries impacted by microbiologically influenced corrosion (MIC) expend millions of dollars either for understanding MIC mechanisms or mitigation of MIC. In MIC, interplay of microorganisms, metal and surrounding environment results in corrosion. Microorganisms exist as biofilms attached to the corroding metal at the sites of MIC. Since there is no single mechanism for MIC, understanding mechanisms and the mitigation strategies should be oriented towards site-specific evaluations. Microfluidic microbiologically influenced corrosion (M-MIC) models were developed that can be used for investigation of mechanisms and development effective mitigation strategies. These models consist of a metal coated glass slide bonded to a transparent polymer imprinted with a rectangular micro-flow channel. Some advantages of the continuous flow M-MIC models are capabilities for real-time monitoring and high-throughput testing in addition to minimal reagent usage. For investigation of MIC mechanisms, the model uses two electrode system with corroding metal and non-corroding metal electrodes in parallel. This enables investigation of the biofilm growth, corrosion mechanisms and indicators of corrosion on metal surface using confocal laser scanning microscopy (CLSM), electrochemical impedance spectroscopy (EIS), and scanning electron microscopy (SEM). For development of effective mitigation strategies, a modified version of the model has been developed such that instead of two different metals there is only one metal (corroding metal). This allows evaluation of biofilm viability grown either from field inocula or laboratory cultures to biocide treatments on the corroding metal surface to determine biocide effectiveness. To summarize, these M-MIC models can be used to non-destructively and simultaneously monitor biofilm development and corrosion mechanisms on metal surfaces both for laboratory and field applications to better investigate and mitigate MIC.

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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]

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

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[3] *Chemical Engineering Department, Texas A&M University at Qatar, Doha, QATAR*

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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[2] *Texas A&M Energy Institute, Texas A&M University, College Station, TX*
[3] *Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ*
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]

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

[2] *Texas A& Energy Institute, Texas A&M University*

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

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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[2] *Dow Chemical Company, Freeport, TX, 77541*

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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[2]*School of Pharmaceutical Science and Technology, Tianjin University, Tianjin 300072, China.*

[3]*Department of Chemistry, Texas A&M University, 3255 TAMU, College Station, TX*
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]

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[2] *Department of Materials Science and Engineering, Texas A&M University, College Station TX 77843*

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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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]

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[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]

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

[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*
[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

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

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

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:

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

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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

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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.