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SCI America

Innovation Day Poster Session Guide

September 12, 2023

Online Poster Session, 9:00 AM – 10:00 AM

In-Person Poster Session, 10:15 AM – 11:15 AM

On Innovation Day emerging industry leaders celebrate today's innovations in the chemical industry and seek solutions for tomorrow's challenges. By taking early-career scientists out of the lab and giving them broader access to their colleagues and to the historical and social context of their research, Innovation Day supports a 21st-century chemical enterprise that addresses society's most pressing needs. Cohosted by the Society of Chemical Industry (SCI) and Science History Institute since 2004, Innovation Day 2023 is a hybrid event held in person and online on September 12. In its 20th year of highlighting breakthroughs and achievement in innovation, our program continues to attract leading speakers and participation from across all sectors of the chemical enterprise.

Innovation Day 2023 features 18 posters. The theme of this year's event explores sustainability with particular focus on life cycle analysis, biomaterials and bioprocessing, and plastics recycling.

This Poster Session Guide is organized alphabetically by poster presenter last name. The Guide includes poster presenter name(s), poster authors (when available), company affiliation, and poster title and abstract for each poster. Please use this as a guide as you prepare to explore posters during the virtual or in-person poster sessions on September 12.

For full poster citations, please contact the poster presenter(s) during Innovation Day 2023.

Presenter Name: Mohammed Abutaqiya
Authors: Mohammed Abutaqiya and Bennett D. Marshall
Company: ExxonMobil Technology and Engineering Company
Poster Title: An Advanced Equation of State for Predictive Modeling of Molecules with Complex Energy Scales

Abstract:
As the energy industry moves towards processing renewable feeds and introducing new chemicals to the market with complex interaction energies, the need of a predictive thermodynamic model is becoming more and more invaluable for early process scoping as well as process development and optimization. We present an advanced equation of state (EOS) model based on the Perturbed Chain Statistical Associating Fluid theory (PC-SAFT) which is capable of accurate representation of the complex interaction energy scales that are frequently encountered in the energy industry such as polar interactions and hydrogen bonding for small and large molecules. A strategic use of the polar free energy term within the proposed EOS framework allows for the accurate description of molecules with unsaturated double and triple bonds such as aromatics, olefins, and alkynes in a fully predictive manner. Additionally, a proper description of the hydrogen bonding tendency of alcohols and oxygenates allows for predictive modeling of, e.g., key properties for alcohol-blended gasoline. We present the theory and a few case studies for the successful implementation of this advanced EOS model.

Presenter Name: Joseph Accardo
Authors: Joseph Accardo[1], Rachael Smith[1], Allyson Marianelli[2], Samantha Woodfin[2], Brian Einsla[2], Melinda Einsla[1], John Roper III[2], Sharon Vuong[1]
[1]Core Research and Development, The Dow Chemical Company, 400 Arcola Road, Collegeville, Pennsylvania 19426. [2]Dow Coating Materials, The Dow Chemical Company, 400 Arcola Road, Collegeville, Pennsylvania 19426
Company: The Dow Chemical Company
Poster Title: Effects of dye formulation on defect detection in waterborne barrier coated papers

Abstract:
The use of paper for packaging is a promising avenue toward greener materials. Unfortunately, the porous nature of paper makes it naturally susceptible to solute permeation. To overcome this, the application of barrier coatings (such as of waterborne polymers) is often employed such that the necessary solute resistance is achieved. Unfortunately, the application of a coating does not guarantee a high-performance packaging, as microscopic structural defects, such as pinholes, cracks, and blistering can dramatically reduce the performance of the barrier coating. As these structural defects are not easily identifiable, the quality of the coating can be inferred from time consuming coating performance tests, such as oxygen or water vapor transmission rate or oil and grease resistance. Consequently, there has been a need to develop tests which can assess the coating quality both rapidly and reliably. This presentation highlights a dye-penetration test used to screen for barrier coating defects and summarizes our efforts to understand how experimental parameters in influence the test results. Our investigation focuses on the performance of two reported dye tests which differ in their dye color (structure of chromophore) and formulation (carrier solvent) on a variety of papers coatings on both freesheet and glassine paper.

Presenter Name: Ashley Childress
Company: Eastman Chemical Co.
Poster Title: The Power of Experimental Design in Innovation
Abstract:
Statistical Design of Experiments (DOE) drives innovation by providing optimized solutions while gaining essential causal information of system behavior. DOE empowers scientists and engineers to make data-driven and defensible decisions, optimize processes and products, and drive improvements. DOE methodologies have evolved to offer highly customizable, flexible, and efficient designs that maximize the extraction of valuable information from a minimal number of experimental runs, aligning with the specific goals of the study. Additionally, these methods work synergistically with AI and machine learning approaches that aim to identify new and improved materials by helping to navigate and provide improved coverage in complex spaces and improve model precision as well as establishing cause-effect relationships. This integration has opened new avenues for predicting and accelerating the development of novel and enhanced materials, streamlining the discovery process, reducing time and resource requirements, and driving breakthroughs and innovation in the chemical industry.

Presenter Name: Brian Edwards
Authors: Collin Ward, Anna Walsh, Taylor Nelson, and Christopher Reddy – Woods Hole Oceanographic; Mounir Izallalen, Sharmi Mazumder, Michael Mazzotta, Steve Perri, and Brian Edwards – Eastman
Company: Eastman Chemical Co.
Poster Title: Rapid Degradation of Cellulose Diacetate Materials in the Coastal Ocean
Abstract:
The pervasiveness of plastic debris in the world's oceans, together with rapidly increasing consumer demand for plastics, has generated intense interest in materials with sustainable characteristics and low environmental persistence. Cellulose diacetate (CDA) is a primarily bio-based material (derived from wood pulp) that is widely used in consumer goods and is proposed to have low persistence should leakage into the natural environment occur. Previous studies have shown that CDA is biodegradable in a variety of environmental compartments, but no peer-reviewed study had assessed the persistence of CDA-based materials in the coastal ocean. In this study, we investigated the degradation of CDA-based materials, alongside positive controls with high degradative capacity and negative controls with low degradative capacity, by marine microbes using a continuous flow seawater mesocosm. Time-lapse photography, cumulative mass loss measurements, and probes of biofilm enzymatic activity indicated that CDA-based materials are susceptible to disintegration and biodegradation by native marine microbes on timescales of months. Shifts in the isotopic composition of seawater dissolved inorganic carbon during short-term bottle incubations confirmed respiration of CDA to carbon dioxide. Collectively, our findings demonstrate that CDA is a high-utility, bio-based material with low environmental persistence.

Presenter Name: Erica Frankel
Company: Dow
Poster Title: Towards More Sustainable Architectural Coatings: Synergistic Design of Biobased Binders for Improving the Carbon Footprint of Premium Architectural Paints
Abstract:
The drive towards sustainability and a more circular economy has become a key strategy across all industry segments and led to a refocus of innovation programs including coatings. In the wake of the

Green New Deal, the paint industry is pursuing various routes to deliver more sustainable coatings. Key practices involve reducing of carbon emissions, leveraging materials with longer usable lifetimes, and sourcing from renewable feedstocks, namely biobased. Presently, biobased coatings are challenged by a mismatch of higher cost without meeting the key performance requirements of a traditional premium paint prepared from conventional petroleum-based emulsions. Herein, we describe several examples of how Dow Coating Materials has been at the forefront of sustainability through directed design of materials that lower the overall carbon footprint in architectural coatings. Moreover, examples will be provided on the development of the first all-acrylic biobased binder for the North American market. Overall, these learnings provide paint manufacturers expanded formulating capabilities when using low-VOC, pure acrylic biobased emulsions, which deliver premium performance attributes that match or exceed conventional petroleum-based binders.

Presenter Name: Adam Gross
Company: ExxonMobil Technology and Engineering Company
Poster Title: Advanced Recycling of Polyolefins
Abstract:
Advanced recycling offers a potential route for the valorization of plastic waste that can help facilitate a plastic circular economy. For polyolefins such as polyethylene (PE) and polypropylene (PP), one method of accomplishing this is via pyrolysis, which yields a complex mixture of products that can be further processed and upgraded for use in or as end products. In this poster, we discuss various aspects of practicing polyolefin pyrolysis at scale. We emphasize the interplay between different fundamental phenomena in the process such as intrinsic chemistry, heat and mass transport, and phase behavior and mixing, which should be accounted for when designing a plastic pyrolysis system at scale. Various factors can affect the pyrolysis system and operations, such as reactor design, operating conditions, and use of catalysts, which are highlighted. Finally, different aspects of feed quality and contaminant types are shared, and the potential challenges and opportunities that come with them are discussed.

Presenter Name: Vince Herrera
Company: DuPont
Poster Title: From Ideas to Action: DuPont's Journey in Harnessing the Power of Generative AI
Abstract:
DuPont's poster highlights the impressive progress being made in leveraging generative AI to address complex business challenges across its operations. The poster details DuPont's journey in harnessing the power of AI, starting from ideation to the implementation of these solutions in real-life scenarios. By leveraging AI, DuPont has been able to transform traditional business processes, including IT support, plant historians, patent searches, and sustainability insights, driving significant productivity gains across operations. The solutions discussed in this poster all aim to provide new insights and opportunities, reinforcing DuPont's reputation as a leader in innovation and technology. Productivity gains from these solutions can result in better identification of inefficiencies, reducing downtime and accelerating R&D while increasing sustainability. The use of generative AI helps DuPont to remain at the forefront of innovation, continuing to provide exceptional products and solutions to those it serves.

Presenter Name: Natalie Kadlubowski
Company: DuPont
Poster Title: Vespel® Enables Longer Service Life and Enhances Performance in Hydrogen Applications

Abstract:
As hydrogen continues to be adopted as a clean fuel of choice, it brings with it a set of uniquely challenging application conditions and technical specifications that must be met. The design engineer must select materials to solve familiar sealing, wear, and friction problems while also contending with cryogenic temperatures, elevated pressures, and the unique physical and chemical characteristics of hydrogen. Specified in extreme application environments to solve these problems for decades, Vespel® polyimides were tested against engineering polymers including PEEK and PCTFE in properties of interest in designing for hydrogen service; hydrogen permeability, compressive modulus, and compressive strength to determine seal integrity, creep to provide an indication of service life, and wear and friction performance in a hydrogen atmosphere to estimate time between maintenance cycles. These studies show a consistent trend: that Vespel® polyimides are well-suited to continuous usage in the extreme conditions common in hydrogen generation, storage, and consumption, and that Vespel® is able to outperform other engineering polymers by both enhancing wear and friction performance and lengthening part service life.

Presenter Name: Corey Kaminsky
Company: ExxonMobil Technology & Engineering Company
Poster Title: Oxidative Stability of Amine-based Sorbents for CO2 Capture

Abstract:
The development of new solid materials for CO2 capture is challenging and no one class of materials will be suited across the diverse CO2 streams comprised of point source and direct air capture applications. However, amines in various forms (liquid, solid-supported) are considered lead materials for both applications. Yet amines are oxidatively unstable and both point source and direct air capture streams contain significant concentrations of O2. This poster presents efforts to quantify the rate of oxidation and identify the products of supported polyethylenimine (PEI) sorbents. We investigated two different supports with and without the addition of a stabilizing agent through use of ex situ NMR and in situ FT-IR measurements on the active materials. We find a minimal impact from support across techniques. The impact of the stabilizing agent is not consistent across spectroscopic techniques, despite the clear enhancement in stability observed for CO2 capacity as a function of oxidation time. These results highlight the challenges inherent to studying a complex material such as PEI and the need to design more oxidatively stable amines for CO2 capture applications.

Presenter Name: Mu Sung (Matt) Kweon
Authors: Mu Sung Kweon[1], Mahmoud Embabi[2], Steven Mendoza-Cedeno[2], Eric S. Kim[2], Patrick C. Lee[2], Anvit Gupta[1], Maksim E. Shivokhin[1], George Pehlert[1]
[1]ExxonMobil Technology and Engineering Company, 5200 Bayway Drive, Baytown, TX 77520 [2]Multifunctional Composites Manufacturing Laboratory (MCML), Department of Mechanical and Industrial Engineering, University of Toronto, 5 King's College Road, Toronto, ON M5S 3G8, Canada
Company: ExxonMobil Technology and Engineering Company
Poster Title: Seeking a Sustainable Future through Lightweighting: Foaming Capability of ExxonMobil High-Melt-Strength Polypropylene

Abstract:

The pursuit of materials that can offer sustainability benefits has become a major focus in various industries to help address value chain sustainability commitments. Among these materials, polypropylene (PP) stands out as an ideal candidate for a wide variety of applications. A prime example of how PP can offer sustainability benefits is its use in plastics foaming. The lightweight nature of PP foams can translate into lower material consumption and the potential for reduced transportation energy, and enhanced fuel efficiency – thus potentially offering carbon footprint benefits in automotive and packaging applications. In addition, the strong chemical resistance and excellent insulation properties of PP foams can result in durable products with long lifespans that can offer energy efficiency benefits in construction applications. However, PP typically possesses low melt strength and produces low-quality foams with poor cell structure, limiting its use in high-density foams. To help address these drawbacks, ExxonMobil has developed high-melt-strength (HMS) PP grades that can deliver significant weight reduction while maintaining the desirable attributes after foaming. In this work, we examined the foamability of these HMS PP materials under conditions relevant to foam manufacturing processes to demonstrate the use of PP foams in various applications.

Presenter Name: Manjiri Moharir
Company: ExxonMobil Product Solutions
Poster Title: Better Call SOL for FCC Operation
Abstract:
The poster presents an introduction to the structure-oriented lumping (SOL) technology for capturing complex reaction networks and its adoption for the operation and optimization for the fluidized catalytic cracker (FCC) units in ExxonMobil. Brief details of an extension to the FCC SOL model to coprocessing of new feeds are also discussed.

Presenter Name: Michael Petr
Authors: Stacey Saba[1], Roshan Aarons[2], Saurav Sengupta[1], Jeffrey Cogen[1], Yabin Sun[3], Edit Berczi[4]
USA[1], Germany[2], China[3], Switzerland[4]
Company: The Dow Chemical Company
Poster Title: Material Developments in Polyethylene Insulated Power Cables for More Sustainable Power Delivery
Abstract:
Population growth and urbanization are leading to substantial increases in energy demand. Energy produced at energy generation sites needs to be delivered to substations and customers via transmission and distribution power cables. Polyethylene-based insulation is widely used in these applications because of its low permittivity, low dielectric loss, and good balance of mechanical toughness, chemical and moisture resistance. Polyethylene-based insulation is crosslinked to increase the temperature rating or ampacity of the cable, where peroxide-based crosslinking is the dominant chemistry for medium voltage distribution and high voltage transmission cables. Peroxide crosslinking is highly compatible with the cable manufacturing process, however undesirable byproducts from the peroxide crosslinking reaction, such as methane, need to be removed prior to completion of the finished cable. This presentation will cover alternative approaches to crosslinking chemistries that were developed to reduce the generation of byproducts in cable manufacturing. We show that the new crosslinkable insulation provides a significant reduction in peroxide decomposition byproducts that are released to the environment, while maintaining the excellent mechanical and dielectric properties of a crosslinked polyethylene. This more sustainable

solution results in an 80% reduction in degassing time and emissions, due to additional material and energy savings.

Presenter Name: Agostino Pietrangelo
Company: ExxonMobil Product Solutions
Poster Title: Morphology, Thermal Behavior, and Toughness of Poly(β-butyrolactone-co-β-valerolactone) Thermoplastics

Abstract:
Mapping copolymer properties to composition and microstructure enriches our understanding of how these features are correlated and establishes a pathway to tune the structural characteristics of the material to meet the performance demands of its end-use application. Here, racemic β-butyrolactone (B) and β-valerolactone (V) are polymerized by ring-opening to afford a series of syndio-enriched (co)polymers that cover the entire compositional range. The effect of copolymer composition on the thermal properties, crystallinity, morphology, and mechanical properties is reported. A monotonic decrease in elastic modulus with increasing V content is observed, with melt transitions following a similar functional form. Tensile properties, including toughness and tensile strength, show sharp transitions at a V content of 36%, coinciding with changes in crystallinity and crystal structure at the same composition. The copolymer microstructure was investigated using 13C NMR spectroscopy enabling a partial assignment of resonances at the tetrad level. The results of this study show that at 27% V content, nearly 50% of the copolymer is comprised of syndiotactic tetrads that have at least three B units. At 36% V content, a significant compositional shift is observed whereby the majority of tetrads are syndiotactic with at least two V units or are iso-enriched.

Presenter Name: Kara Radford
Company: ExxonMobil Product Solutions
Poster Title: Let's Talk Trash: A Discussion on Plastic Circularity

Abstract:
This poster describes the current state of plastic waste recyclability, exploring advanced recycling as a complement to mechanical recycling in driving for increased plastic circularity. This poster discusses the compatibility of plastics 1-7 with both mechanical and advanced recycling and discusses the national challenges facing both technologies. Examples of plastic wastes are shown with a description of the landscape of plastic waste.

Presenter Name: Ali Slim
Company: ExxonMobil Product Solutions
Poster Title: Next generation film design enhances process-to-application sustainability in packaging materials via innovative catalysis and formulation

Abstract:
Sustainability in the packaging world is a complex challenge in modern film design. Ensuring durable materials with high customer satisfaction requires a balance between the everlasting compromise between performance and processability. The conventional way of producing printed films and converting them into packaging materials is prone to variability and human errors. Developing a resin with the right properties can simplify the complexities by providing high performance while enhancing processability. Our recently developed polyethylene grades offer simplicity without compromises on performance. Processers can achieve high levels of toughness and stiffness with less material and blending while

improving durability in a simpler operation. The main advantages are summarized are follows: Sustainability benefits via increased performance and reduced need of polyethylene blending grades for processing; Waste reduction by creating flexible and durable materials for longer lasting packaging; Enhanced packaging efficiency through less extensible films. The benefits of the new generation of polyethylene grades make them very suitable for a multitude of applications including primary packaging, polyethylene laminates, and heavy-duty sacks.

Presenter Name: Laurien Vandewalle
Authors: Kevin Buettner, Timothy Healy
Company: ExxonMobil Technology and Engineering Company
Poster Title: Application of Filtered Two-Fluid Models to Industrial-Scale Fluidized Beds
Abstract:
Gas-solid fluidized beds are known for their enhanced heat and mass transfer characteristics and are therefore widely used in industry to make various chemical processes more efficient. Supported by recent developments in high performance computing capabilities, computational fluid dynamics (CFD) has become an invaluable tool in the study, design and scale-up of gas-solid fluidized beds. The preferred modeling method for industrial fluidized bed applications is the Eulerian-Eulerian approach (i.e., two-fluid model). The two-fluid model with classical drag laws is able to capture the complex multi-scale flow phenomena occurring in gas-solid flows, but to preserve accuracy, the mesh resolution should be limited to ten particle diameters at most, which is impractical for most full-scale applications. By replacing the classical micro-scale drag laws with a meso-scale 'filtered' model, the mesh resolution requirements and hence computational cost can be significantly reduced. The CFD group at ExxonMobil has been using filtered drag models for over a decade. In this presentation, industrial successes in applying these models to refining and chemicals processes will be discussed. Furthermore, we will highlight some challenges that had to be tackled when using the existing filtered models outside their original validation range.

Presenter Name: Megan Witzke
Company: ExxonMobil Technology and Engineering Company
Poster Title: Advanced Materials for Renewable Diesel and Jet Production
Abstract:
Here we will discuss the ExxonMobil's work in developing technologies for lower-emission fuels through advanced dewaxing technologies that maintain higher yield of renewable fuels with greater cloud point improvement along with lower H2 consumption. ExxonMobil Renewable Diesel (EMRDTM) with BIDWTM provides pathways to upgrade bio-feedstocks including vegetable oils, unconverted cooking oils, and animal fats into renewable diesel with the option of generating renewable jet. Advancements in hydroprocessing enabled by continued materials development will aid in meeting aviation and diesel fuel demand with lower-emission fuels.

Presenter Name: Alex Zabula
Company: ExxonMobil Product Solutions
Poster Title: Towards the Next Generation of General Purpose Rubbers: Polypentenamers
Abstract:
Controlled ring opening metathesis polymerization (ROMP) for cyclic olefins is a powerful platform for the development of new types of elastomers with improved properties including polymer-to-monomer circularity. This work discloses controlled ROMP of cyclopentene (CP) alone, or with

dicyclopentadiene(DCPD) for the production of long chain branched polypentenamers. The variation of ligands at the metal catalytic center was used to control cis/trans ratio, molecular weight and molecular weight distribution of the resulting polymers. This invention paves the way to the development of entirely new GPRs with controlled architecture and remarkably improved attributes (e.g. melt strength, shear thinning, and tensile strength) which brings value for various tire applications. Finally, the resulting elastomers exhibit potential for selective conversion back to monomer under mild conditions using Ru-based catalysts in the yields above 90%.