SURFACTANTS AND DETERGENTS

S&D 1a: Fabric Care

Chair: Yvon Durant, Itaconix, USA

Formulating High Performance Odor Neutralizing Carpet Cleaners. Gregory Smith*[1], Scott Jaynes[1], and Anita Augustyniak[2],[1]*Croda, Inc., USA;* [2]*Itaconix, USA*

Carpet cleaning shampoo formulations must deliver high cleaning performance, appropriate foaming levels, and low residues after cleaning. In addition, cleaning formulations should neutralize persistent odors such as those from pet stains, food and smoke whether in household or institutional settings. Finally, market demands for sustainable products mean that these cleaning products must incorporate highly renewable raw materials that have acceptable toxicity and biodegradation profiles. We present guidelines for producing carpet cleaning formulations that meet these high performance standards using highly sustainable raw materials. Cleaning surfactants are chosen from a family of high bio-based materials with EPA Safer Choice® and USDA BioPreferred® credentials. Odor neutralization is provided by zinc polyitaconate, an effective, water soluble and bio-based odor neutralizer. Data will be presented showing the high performance and low residual material left behind by these formulations, as well as potential negative effects from residuals of alternative odor neutralizers such as zinc ricinoleate.

Deliver In-Wash Laundry Care with Minimal Greying - Smart Cationic Sensorial Enabler. Yunshen Chen*, Randara Pulukkody, Emmett Partain, John Hayes, Peilin Yang, Michael Clark, Sharon Vuong, Daniel Miller, Asghar Peera, and Mariann Clark, *Dow Chemical Company, USA*

Cleaning is a primary need when doing laundry. While today's consumers do not want to compromise on cleaning, there is increased interest in products that offer sensory benefits in addition to cleaning. Leveraging sensorial attributes related to touch and smell enable enhanced consumer enjoyment while doing laundry and benefit from an extended sensorial experience after laundering provided by innovative multifunctional sensorial ingredients. One of the key challenges for such multifunctional sensorial ingredients for use in 2-in-1 automatic laundry detergent is the delivery of a fabric care benefit through the wash while minimizing compromise on whiteness retention. Current multifunctional sensorial ingredient technologies typically lead to excessive greying and loss of color brightness of fabrics. Our new cationic cellulosic additive addresses this challenge by offering improved softness and fragrance deposition with minimal greying negatives that renders the experience of doing laundry more enjoyable.

Study on Change in Clothing Texture of Clothes Bought by Depending on Drying Method. Hiroyuki Masui, Aiko Tai*, Shota Okeda, Tsuyoshi Terabayashi, Ai Tanaka, Yoichiro Kohno, Yukari Matsunaga, Lion Corporation, Japan

As more Japanese women choose full-time employment over staying at home and pollen, PM2.5, etc. deteriorate the outdoor environment, drying laundry indoors is becoming more common. However, our research shows that most Japanese consumers still want to dry outdoors, and even those who own dryers may seldom use them. One major reason is that consumers expect drying outdoors to not only dry their laundry completely and eliminate odors but also make it feel good. In this study, we focused on laundry texture after outdoor drying as a new value and

looked at how to achieve it indoors. First, we interviewed consumers and found fluffiness and dryness to be important factors for them. We evaluated the physical properties of towels dried under a variety of conditions and discovered that compared to indoor drying, towels dried outdoors were thicker and transferred less heat. Postulating that this was because the greater thickness contained more air, reducing heat transfer, our research then revealed a positive correlation between fluffiness and thickness and a negative correlation between dryness and heat transfer. In other words, wind and the sun's heat raised the towel piles, increasing fluffiness and reducing heat loss when touched, increasing the feeling of dryness. Based on these findings, we studied how to chemically impart physical properties to fabric and found that increasing and maintaining fiber bulkiness created the feeling of outdoor drying even when dried indoors. Finally, we explored what kinds of affective values that this dried-outdoors feeling provides consumers.

Elucidation of Softening Mechanism in Rinse Cycle Fabric Softeners. Takako Igarashi*[1], Masato Hoshi[1], Kouichi Nakamura[2], Takeshi Kaharu[2], and Ken-ichiro Murata[3],[1]*Kao Corporation, Japan;* [2]*Material Science Research Laboratory, Japan;* [3]*Institute of Low temperature Science, Hokkaido University, Japan*

We have proposed a new idea that softening mechanism with the use of fabric softener that softener has an important role of inhibition of constructing 3D cross-linkage of hydrogen bonding network made of non-freezing type of bound water. We have understood the detail of effect of softener to this kind of bound water with new surface analytical method.

S&D 1b: Trends in Clothing/Trends in Machines

Chairs: Erika Szekeres, Method, USA; and Hongwei Shen, Colgate Palmolive Co., USA

Principles and Applications of PhabrOmeter - Comparison with Other Existing Instruments Ning Pan*, *University of California Davis, USA*

This talk starts by examining the physics of fabric sensory performance including the tactile (Fabric Hand) and visual (Wrinkle Recovery and Drape) properties, and the challenges in measuring them. It will also explain the inherent problems in other existing instruments. Then the principles of PhabrOmeter design and operation will be introduced. Through both analysis and practical applications, it will demonstrate why PhabrOmeter is indeed a promising technology for measuring and evaluating fabric sensory properties. Focuses will also include issues like the repeatability or reproducibility; sensitivity or resolution of the instrument; range of product coverage (density and thickness) and types of products (woven, knit, nonwoven, tissue, etc.), as well as the applications (both proved and potential) of the technology for cloud data analysis and online service to industries and consumers. Test results of samples from various users are provided as examples.

Impact of ADW Machine Design on Formulations and Raw Materials Jim W. Gordon*, and Bo Jiang, *Itaconix, USA*

European and North American dishwashers have noticeable differences that when combined with market preferences and testing methodology differences results in quite different formulations. Institutional and commercial machines are different again as consumer dishwashers take too long to complete a wash cycle. In this sector machine size and detergent solubility matters. Products tend to be in a Liquid format for small machines and in Liquid or Solid block format for larger and more expensive units, placing a different set of challenges on the formulator. Examples will be given how polymer design can affect both the physical properties, such as tableting, and the performance of dishwash cleaners in the consumer and Commercial sectors in order to illustrate how formulators respond to machine and market differences. Other formulation adjustment reflecting the trends in water conservation, lower temperatures, shorter cycle times impact will be discussed, particularly regarding total soil load, and soil removal.

Dishwashing Appliance Trends' Impact on Detergent Formulation Monica Ochoa Ruiz*, *Home and Personal Care, DuPont, The Netherlands*

The dishwasher appliance industry is focusing on improving the consumer experience of using a dishwasher and solving unmet needs, together with detergent manufacturers and other stakeholders in this industry. In the 1960's, the 'Sinner circle' concept was developed, stating that cleaning performance is a function of time, temperature, mechanical action and chemistry. Therefore, if one component is decreased, one or more of the other factors must increase to compensate for it, meaning that dishwashing appliance trends such as reducing the cycle length or main wash temperature, can have a significant effect on innovations for detergent formulations. The key Dishwashing appliance trends are providing solutions for convenience, performance and sustainability. By way of illustration, dishwashing appliance manufactures in North America are looking at decreasing the cycle time to help consumers to keep their fast pace while reducing their impact to the environment. Therefore, the new energy efficient automatic dishwashing machines have a short cycle option for which the detergent contribution must

compensate and enzymes are key ingredients to address these new challenges. These developments create new opportunities for innovation in ADW detergents to deliver on performance expectations under new conditions.

Sustainable Fabric Protection using Bio-Polymers Gregory Smith*[1], Sue Burn[2], Scott Jaynes[1], and Xin Chen[1], *[1]Croda, Inc., USA; [2]Croda International Plc, United Kingdom*

An effective way to provide sustainability to laundry consumers is to minimize damage to fabrics in the washing and drying process so that garments last longer and need to be replaced less often. This is particularly true for high value garments that incorporate engineered fibers, surface treated materials, and highly colored synthetic and blended fabrics. We present a bio-polymer based additive for fabric softeners that provides measurable improvements in fabric protection compared to the use of traditional fabric softener alone. The bio-polymer is highly substantive to textile fibers, delivering colour protection, reduced greying of whites, and reduced damage to fabrics through multiple washing and drying cycles. As a result, fabrics are kept looking newer for longer, reducing the need to replace garments. We will present a quantification of the water savings and reduced emissions offered through this lifetime extension of garments.

S&D 1.1: Analytical and Performance Determination

Chairs: Robert Nolles, Cosun Biobased Products, USA; and Eric Theiner, Evonik Corporation, USA

Wettability Determination using High-Speed centrifuge, NMR, and Micro-CT Sarmad Khan [1], Syed S. Hussain[2], Muhammad Sha Kamal*[2], Xianmin Zhou[1], and Syed S. Hussain[2],*[1]KFUPM, Saudi Arabia; [2]King Fahd University of Petroleum and Minerals, Saudi Arabia*

The primary objective of this study is to assess the wettability alteration of different rocks by injection of different commercial surfactants using a high-speed centrifuge, NMR, and micro CT. This is done by determining drainage and imbibition capillary pressure curves of an oil/ water system and then doing the same with an oil/surfactant system. Three different surfactants from different classes were studied and two different rocks were used. The drainage and imbibition tests are conducted on a centrifuge where the core samples immersed in a mobile injection fluid are spun at predefined speeds for a certain period. NMR and micro CT were also used to study the wettability alteration and results were compared with the centrifuge. The USBM wettability index obtained from high-speed centrifuge was used to measure wettability alteration of different rock types. Results obtained using different surfactants and rocks reveal that wettability alteration strongly depends on surfactant type, rock type, and aging process. The hydrocarbon zwitterionic surfactant was most effective to alter the wettability of the Indiana limestone from oil-wet to neutral-wet and water-wet, followed by fluorinated zwitterionic surfactant and fluorinated nonionic surfactant. The micro-CT data and NMR data also supported the wettability alteration data obtained using a high-speed centrifuge. This work is first of its kind where wettability alteration was studied by a combined approach using a centrifuge, micro CT, and NMR analysis. This comprehensive approach will lead to a more reliable understanding of rock-fluid interactions.

Branched Alcohols Contribution to Surfactants Characteristic Curvature and Other HLD-NAC Parameters Sanja Natali*, *ExxonMobil Chemical, USA*

The HLD-NAC methodology is increasingly being used for surfactants formulations, creating opportunities to fine tune molecules and optimize performance for numerous applications. To that extent, a series of branched alcohol ethoxylates were evaluated with the goal of obtaining contribution of alcohols to characteristic curvature and characteristic length of surfactants. Surfactants with different tail lengths, ranging from C8 to C13, and different degrees of ethoxylation were examined with salinity scans at different temperatures. Additionally, free alcohol effect was studied to provide complete characterization of these molecules. The detailed results will be presented and the data analysis will be discussed.

MACH 5+, the Next Generation of Image Analysis for Measuring Cleaning Performance Caspar van Leeuwen*[1], and Björn Hotting[2],*[1]Center For Testmaterials BV, Netherlands; [2]Colour Consult BV, Netherlands*

Six years ago the MACH 5 was introduced in the detergent industry. A Multi-Area Colormeasurement Hardware. The MACH 5 was designed to save time in assessing the results of any wash performance test, especially in combination with multi-swatch monitors. The use of image analysis tools and software is getting more common in our industry. The MACH 5 is the only instrument developed from within this same industry and thus its is particularly equipped for use in testing laundry

detergents, (auto)dish detergents, and other cleaning agents. With the introduction of the new MACH 5+ even more accurate L*A*B* and XYZ measurements can be generated, where the user is free to position as many 'sample areas' as needed on a 27x35cm measurable area and assess the results for all of these sample areas simultaneously in only a few seconds. The biggest improvement is that the MACH5+ can give %R reflection values in 10nm intervals similar to a spectrophotometer. This makes the difference between a conventional spectrophotometer and this image analysis device even smaller. Another improvement is the gloss-reduction filter which gives better measurements for glossy objects, like dishes, glass, stainless steel etc. Apart from the timesaving advantage, the device is also very capable in measuring non-homogeneous surfaces, which is often necessary for dish wash and hard surface cleaning tests. Compared to the MACH5, the MACH 5+ has enhanced light sources which yield more accurate measurements across the entire visible spectrum and more homogeneous lighting over the measurable area.

Employing Image Analysis to HLD-NAC Salt Scans Eric Theiner*, and J. R. Bennett, *Evonik Corporation, USA*

As the use of the HLD-NAC model in formulation gains momentum, there is increasing interest in characterizing surfactants in terms of Characteristic Curvature (Cc) and hydrophobic materials in terms of Equivalent Alkane Carbon Number (EACN). Although calculations can be used to give initial indications for these values, experimental evidence is the only way to ensure the correct values are used. This becomes even more necessary when industrial grade, rather than pure, materials are being examined. The experimental method, often called a salt scan, is simple but time consuming. Screening (i.e. narrowing an experimental field to pinpoint a value) often requires multiple iterations as well. This presentation will show how the use of a robotic formulator, combined with image analysis, can simplify salt scans and provide data that will minimize screening runs with proper analysis.

Comparing Industry Soiled Stains to Freshly Soiled Stains in Laundry Detergent Evaluations Tod Losey*, *Sterling Laboratories, USA*

Objective: To show differences in the soil removals that may or may not be valuable to detergent manufacturers when determining levels of performance

Methods Used: Consumer Washers, Average Wash Conditions (120ppm water/90°F wash temperature). ASTM D4265 & D3050-Based Methodologies used as guidelines for testing.

Results: Results will be given in % Soil Removals based on Reflectance Values of the swatches, before & after testing. Comparisons of the detergents used will be broken down by soil groups and over all soil removals
Conclusions: Conclusions will discuss the differences found between the 2 stain sets. Positive and negative outcomes will be discussed.

Effect of Alkyl Chain Distribution, Branching and Oligomer Distribution on Hard Surface Cleaning Performance George A. Smith*[1], and Ollie James[2], *[1]Sasol North America, USA; [2]Sasol Performance Chemicals, USA*

The effect of nonionic surfactant structure on cleaning performance of oily particulate soil using in-line abrasion testing has been investigated. Soil removal was measured as a function of cleaning cycles to give kinetic curves describing the cleaning process. The effect of alkyl chain length, different kinds of branching in the hydrophobic chain, the degree of ethoxyaltion and peaking of the oligomer

distribution has been studied. The alkyl chain length was varied from C6 to C20. Different types of alkyl chain structures were studied including linear, C2 monobranched, random chain branching and multiple methylbranched hydrophobes. The degree of ethoxylation was varied to span a range of HLB values and the oligomer distribution was also peaked using a narrow range alkoxylation catalyst. Dynamic interfacial tension between surfactant solution and soil components was measured by drop volume and correlated with soil removal. Soil removal depends on a number of different factors. In general, soil removal increases with decreasing alkyl chain length. Shorter chain lengths give lower IFT values and faster wetting kinetics. Soil removal increases with increasing branching in the hydrophobe. Branching at the C2 position lowers the effective chain length and lowers IFT values. The optimum degree of ethoxylation depends on the alkyl chain length. For the oily particulate soil studied, the optimum surfactant HLB is around 11. Peaking the oligomer distribution decreases IFT and improves soil removal. Learning's can be used to formulate better hard surface cleaners for different applications.

Limiting Variance: Exploring Primary Cleaning Evaluations for Hard Surface Cleaners Kevin M. Salmon*, *BASF Corporation, USA*

In this presentation, best practices of primary cleaning evaluations for products intended for use on assorted hard surfaces will be explored along with a critical assessment of the currently implemented industry standards. Method parameters (e.g., substrate selection and preparation, soil composition and application techniques, mechanical action, etc.) were trialed under controlled, but practical, hard surface cleaning conditions to optimize for differentiation. Once key factors were determined, the method was challenged for precision and accuracy. Market trends in hard surface, performance data with detailed analysis and method parameter recommendations will be presented.

The Interaction of Hydrophobe-Terminated Nonionic Surfactants with Silica Eric P. Wasserman*, Kebede Beshah, Sara Klamo, Junsi Gu, Fang Yuan, and Robert Campbell, *The Dow Chemical Company, USA*

Low cloud-point nonionic surfactants are often included in automatic dishwashing detergent formulations to improve the appearance of glassware and other surfaces. Analytical and computational techniques were brought to bear on a series of capped surfactants with varied ethylene oxide (EO) and 1,2-epoxybutane (BO) block lengths in order to evaluate how they function in wash liquor of varying temperature. Clouding out, an endothermic phenomenon, is surprisingly uncorrelated with significant changes to the local environment of the surfactant molecules as viewed by NMR. At low surfactant loadings, silica suppresses the signal from the EO blocks to an extent that defies explanation by fractionation, and indicates that the initial monolayer is strongly anchored by hydrogen bonds. Molecular dynamics simulations indicate that both EO and BO blocks can participate in hydrogen bonding to an amorphous silica surface. However, robust multilayer structures form at higher surfactant:silica ratios, and this process appears to be endothermic overall. Thus BO appears to have a dual nature: hydrophobe and promoter of adhesion to surfaces with active protons.

S&D 2a: Trends in I&I Cleaning and O&G Applications

Chairs: Michael Tate, The Dow Chemical Company, USA; and Juan Goncalves, Diversey, Inc., USA

Globally Harmonized System (GHS) Trend for I&I Cleaners: Surfactants to Help Minimize GHS Pictograms and Classification Ron A. Masters*, Lela Jovanovich, Tracy Strilich, Luke Jancich, and Sangeeta Ganguly-Mink, *Stepan Company, USA*

Response to GHS initially was focused on tactical operations, such as updating Safety Data Sheets (SDS) for compliance. Recently, however, a more strategic trend is emerging where manufacturers of cleaning products are seeking formulations with minimal SDS hazard and pictogram designations. Achieving this with concentrated dilutable cleaning formulations can be a significant challenge. This presentation discusses the technical aspects of this challenge with concrete examples focused on the surfactant portion of formulations.

Shiny and Spotless Dishes with Phosphate-free Formulations Yves Kensicher[1], and Alexandra L. Foguth*[2], *[1]Coatex SAS, France; [2]Arkema, USA*

The recent European regulation banning the use of phosphate in automatic dishwashing products forces companies to completely reformulate their product range. To answer this specific need, Coatex has designed a new polymeric dispersant, Rheosolve™ D 15AS, providing outstanding performances of anti-spotting and anti-filming. Rheosolve™ D 15AS is a proprietary product with a unique chemical structure and it has been developed thanks to an innovative technology combining process and chemistry.

C20+ Alkoxylates in Industrial Applications Ollie James*[1], and George A. Smith[2],*[1]Sasol Performance Chemicals, USA; [2]Sasol North America, USA*

Abstract not available.

Ability of Terpene-Based Microemulsions to Remove Asphaltene Residue from Solid Surfaces Eleazar Mendoza[1], Alyssa Perrard[2], Helen W. Hernandez*[2], Wesley Ehlert[2], and Siwar Trabelsi[2],*[1]Texas A&M University, USA; [2]Flotek Chemistry, USA*

Asphaltenes often precipitate and then deposit on the rock surfaces altering the wettability and plugging formation pores with a detrimental effect on relative permeability and oil production. This paper showed the ability of terpene based microemulsions to remove asphaltenic residue from solid surfaces using two novel experimental techniques. One technique is based on the use of microfluidics to visualize asphaltene residue deposition into model two dimensional (2D) porous media followed by application of a dilute microemulsion to wash off asphaltenic residue. The removal is quantified by analyzing images taken before and after microemulsion treatment using image analysis software. Another technique consists of shaken bottle tests to quantify the removal of asphaltenic deposits from crude oil coated sand. In both techniques, the diluted microemulsion removed a significant amount of the residue compared to surfactant alone. The amount of removal was strongly dependent on surfactant chemistry, solvent type and amount contained within the microemulsion as well as microemulsion concentration and crude oil composition. These techniques can be used to effectively quantify removal of asphaltene residues from solid surfaces and to better understand the underlying mechanism of removal. These results are expected to have a significant impact in completing and re-stimulating wells using microemulsions.

Effect of Reservoir Parameters and Surfactant Structures on Surfactant – Rock Adsorption in Various Rock Types Daniel F. Wilson*[1], Laurie A. Poindexter[1], Carla Morgan[2], and Thu Nguyen[2], *[1]Sasol North America, USA; [2]Sasol Performance Chemicals, USA*

Role of both the adsorbent and surfactant molecule are individual characteristics that combine to affect how adsorption of surfactant occurs onto rock surfaces. Surfactant adsorption capacity in crude oil reservoirs is variable and dependent upon a number of unique parameters specific to each reservoir, adding complexity to these relationships. Considering that surfactant based unconventional means to improve oil recovery are strongly dependent on the liquid/liquid interface between soluble surfactant solution and crude oil, loss of surfactant to liquid/solid interfaces can create negative effects for these applications in terms of performance and economics. Alcohol propoxy sulfate and ether carboxylate were the two anionic surfactant types studied. Focus was on investigating static adsorption mechanisms of surfactants onto sandstone, limestone, and shale reservoir media. Besides quantifying how much surfactant is adsorbed, emphasis on the effect of surfactant parameters on adsorption capacity was evaluated. Notwithstanding specific surfactant parameters, a number of other mechanisms involved in surfactant loss from aqueous solutions to varied porous media add to the complexity of this phenomenon. Effects of temperature, pH, and salinity on adsorption capacity of surfactants to solid surfaces also play strong roles. These parameters were isolated and evaluated to determine their influence on static surfactant-rock adsorption capacity. Therefore, this study attempts to investigate effects of reservoir environments, including temperature, formation water pH and salinity on the adsorption capacity of the two anionic surfactant types. This may help enhance designing surfactant molecular structures that minimize adsorption to rock surfaces, while maintaining desired fluid performance for effective oil recovery.

Rapid Identification of Surfactants to Improve Rheological Compatibility and Cleaning of Oil-Based Drilling Muds Carol Mohler*[1], Thiago Alonso[1], Robert Sammler[1], Valeriy Ginzburg[1], Stephanie Hughes[1], Brian Nickless[1], Anatoly Medvedev[2], and Yan Gao[2],*[1]Dow Chemical Company, USA; [2]Schlumberger, USA*

During oil well completion, aqueous-based spacer fluids are used to remove the drilling fluid (mud) from the casing prior to cementing. The spacer is intended to displace the drilling mud from the well, invert the emulsion, and transform casing surfaces from oil-wet to water-wet. However, many mud-spacer mixtures exhibit significant rheological incompatibility, which could generate viscosity spikes and lead to incomplete cleaning. Surfactants may be added to the spacer to promote fluid compatibility and cleaning effectiveness, but it is challenging to screen surfactants for these properties in complex mixtures using conventional rheology techniques. A new approach is described to identify spacer fluid surfactants and solvents that are effective in cleaning and promote rheological compatibility. An automated total aspiration and dispense viscometry method (TADM) is combined with a standard rotor cleaning test to rapidly identify effective surfactants or other additives. The relationship between surfactant properties and rheological compatibility is described, and a model proposed for rheological incompatibility based on the formation of co-continuous phases and disruption by surfactants. The best performing surfactants identified by TADM measurements are further tested for mud cleaning effectiveness using a rotor test. The addition of co-solvent to the spacer formulation further

improves its cleaning ability, and cleaning efficacy is related to solvent properties. The combination of high-throughput technology and rheology gives insight into the viscosity spikes observed in mud-spacer mixtures, and guides new approaches for rheology control and cleaning effectiveness.

S&D 2b: Disinfectants and Preservatives

Chairs: Andrew Guttentag, Church and Dwight, USA; and Nancy Falk, Clorox, USA

Application of Quantitative Microbial Risk Assessment (QMRA) to Predict Infection Risk by Disinfection Interventions of Hard Surfaces Charles P. Gerba*[1], and Nancy Falk[2],[1]*University of Arizona, USA;* [2]*Clorox, USA*

Quantitative Microbial Risk Assessment (QMRA) has been used by the U.S. Environmental Protection Agency and the World Health Organization to set guidelines for treatment standards for drinking water and wastewater reuse. The process involves estimating the risk of infection from a given pathogen via a route of exposure (water, food, fomites). Models based on this process can be used to determine quantitatively the reduction in the risk of infection from interventions (e.g. disinfection of drinking water). QMRA has been validated against epidemiological data involving outbreaks of food, drinking water and fomite transmission. QMRA has been used to determine reduction of risks of infection from hard surface disinfectants and hand sanitizers in homes, office buildings, hotels, nursing homes, and outpatient clinics using tracer viruses. It can also be used to set targets for the reduction of a pathogen on hard surfaces to achieve a certain level of risk of infection. QMRA offers a new tool for setting standards for performance of disinfectants and other hygiene interventions.

Functional Secondary Benefits of Fragrances and Flavors in Consumer Products Charles C. Steward*, *Takasago International Corp. (USA), USA*

Fragrances and flavors are most commonly created and used based on the primary attributes of olfaction and taste. In addition to the sensory properties and benefits of fragrances and flavors, they often have secondary functional activity benefits that can be researched and exploited. These can include antimicrobial activity, product preservation, odor control and even human physiological impacts. We dedicate a significant portion of our research efforts to understanding this functional activity. Primary research tools utilized are microbiology, enzymology, and analytical science. When can see clear opportunity in use when beneficial properties such as preservation are targeted. Fragrances may be able to supplement or replace existing preservatives in a formulation. In addition, in consumer goods for home care applications, needs and opportunities exist for development of fragrances that have antimicrobial activity via kill or inhibition. This activity can be used to supplement product actives, support claims and enhance performance. Other efforts have focused on understanding the positive benefits of fragrances and flavors for odor control based on biological activity. This talk will summarize some of the scientific background of these efforts and provide R&D support for the use of fragrances and flavors to achieve functional secondary benefits in consumer good product applications.

Polymer-micelle Complexes for Enhanced Adsorption and Antimicrobial Activity David Scheuing*, and Nancy Falk,*Clorox, USA*

Quaternary ammonium compounds (quats) are commonly used to provide antimicrobial activity in household and professional cleaning formulations. Antimicrobial efficacy, including kinetic effects, depends on the extent and rate of adsorption of quats onto the complex surfaces of microbes. The formation of mixed micelles of quats and other surfactants can negatively affect the efficacy, due to reduced quat monomer concentrations and/or enhanced binding of quats to cellular debris. Complexes of micelles containing quats with

soluble anionically charged polymers are known to deliver adsorbed layers which are fundamentally different from mixed surfactant adsorbed layers. The utility of this approach to controlling the efficacy of quats will be reviewed.

Beyond the Blindfold – Conquering the Unseen Enemy Gina P. Sloan*, *Microban International, Ltd., USA*

Healthcare Associated Infections (HCAIs) are an increasingly prevalent issue for hospitals, care homes and other healthcare facilities worldwide. Despite the efforts of global public health organizations to raise awareness of the importance of hand hygiene, compliance remains low, indicating the need for additional preventative measures. The patient environment has been highlighted as a potential source of pathogen contamination and transmittance, focused mainly on inanimate objects surrounding the patient. In many cases, infection control (IC) professionals set standards for disinfection regimens but there are limited indirect measuring techniques. This leaves the IC to operate in the blind. How do you know the correct chemistries were used? How can you monitor the cleanliness of multiple surfaces? What new technologies exist to aid in measuring compliance to disinfection regimens? Research has shown that immediate feedback to cleaning crews improves compliance, but this typically takes direct observations or multiple room visits by the IC. A new technology exists that will aid in compliance measurements and immediate feedback loops to create a better outcome for patients.

A Brief Overview of the Continuum of Care: The Cleaning Touchpoints Doe Kley*, *Clorox Company, USA*

This presentation will review the environment in different healthcare settings, from clinic to hospital to long term care. You will learn about the priorities, the staff, and the implications on cleaning and disinfection in the different departments and settings. You will also learn about the staff that makes the decisions on disinfectant selection for different health care settings.

S&D 2.1: General Surfactants I

Chairs: Michael Miguez, Shell Global Solutions, Inc., USA; and Ann Lee, Novozymes North America, Inc., USA

Microemulsions as Robust Electrolyte Solutions for Electrochemistry? Douglas G. Hayes*, Jing Peng, Thomas A. Zawodzinski, Gabriel A. Goenaga, and Mark Dadmun, *University of Tennessee, USA*

The development of energy storage systems that are fast, utility-scale, and power-dense is a grand challenge for the development of robust 21st Century power systems. Microemulsions are one examples of potentially useful nanostructured fluids that can be employed to meet this grand challenge. This presentation will provide a critical assessment of microemulsions' employment in electrochemistry and energy storage, identifying gaps in knowledge based on the current literature. In addition, our initial results will be described. We have investigated oil in-water microemulsions formed by a model system consisting of the electron carrier, (oil-soluble) ferrocene, dissolved in the toluene/Polysorbate-20/butanol/water (electrolyte solution) system for their performance in electrochemistry and their behavior near model electrode surfaces. From cyclic voltammetry studies, we have determined that higher volume fractions of microemulsions provided very high current densities, even though the microemulsions are weakly structured and likely consist of water and surfactant as the continuous phase . From neutron reflectivity studies, we have determined that the structure of the microemulsions changes significantly near surfaces, with the hydrophobicity/hydrophilicity of the surface playing a significant role.

Impact of Number of Ethylene Oxide Groups on the Surface and Thermal Properties of Betaine-based Polyoxyethylene Surfactants for Enhanced Oil Recovery Syed S. Hussain*, and Muhammad Sha Kamal,*King Fahd University of Petroleum and Minerals, Saudi Arabia*

The salinity of carbonate reservoir ranges from 120,000 ppm to 220,000 ppm and the temperature is around 100 oC. The injected surfactants can be degraded due to these high salinity and high temperature environment which ultimately reduce the surfactant ability to lower interfacial tension. The stability of the applied surfactants under such harsh conditions is a challenging task. In order to overcome the stability issues, variety of betaine based polyoxyethylene conventional zwitterionic and gemini cationic surfactants were synthesized. The structures were confirmed using NMR (proton and carbon) and FTIR spectrometry. The short range heat stability was investigated using thermogravimetric analysis and the long range heat stability was studied by aging methods. The interfacial tension was identified using spinning drop technique and surface tension was measured by pendant drop method at 20 oC. The rheological parameters were identified using discovery hybrid rheometer (DHR-3). The synthesized surfactants exhibited excellent short rang and long range thermal properties. The interfacial tension, critical micelle concentration and the related surface tension values were comparable to the commercial surfactants. The rheological results indicated that the storage modulus was reduced by enhancing the concentration of surfactants at low frequency and shear rate because of surfactant polymer interaction and charge screening. The synthesized betaine based polyoxyethylene surfactants showed excellent heat stabilities and salt tolerance and displayed

huge potential in high salinity high temperature carbonate reservoirs.

Secondary Alcohol Ethoxylate - Process and Applications Revisited David Li*,*Jiangsu Secol Chemical Company, China*

Secondary alochol ethoxylates (SAE) are a series of non-ionic surfactants that have been around for more than half a century. Due to limited manufacturing capacity, the applications are limited despite its unique physicochemical and biodegradation properties. Jiangsu Secol Chemical Company (China) will add 18kta SAE capacity in 2019 and 160kta in 2022 with improved process technology and product propeties, e.g. 4~5% higher yield from normal paraffin, narrower EO distribution of high-mole ethoxylates. Combining lower cost and better low-temperature properties, SAE will see wider applications from high-concentration homecare to industrial cleaning. This talk will describe the improved SECOL process technology and demonstrate the improved physicochemical properties of the SAEs thus made.

Surfactant EOR Formulations for High Temperature/High Salinity Reserviors Thu Nguyen*[1], Carla Morgan[1], and Jorge M. Fernandez[2],[1]*Sasol Performance Chemicals, USA;* [2]*Sasol North America, USA*

The challenges of chemical enhanced oil recovery (EOR) formulations for reservoirs with high temperature (HT) and/or high salinity (HS) are often associated with the phase instability of the formulations. Alkyl propoxy sulfates (APS) had been demonstrated to have robust performance in oil/water interfacial tension (IFT) reduction and increased oil solubilization capacity for effective oil recovery. However, at HT/HS, these surfactants tend to precipitate and create phase instability, which can lead to lower oil recovery. Adding appropriate co-surfactants can improve the aqueous stability of APS at HT/HS. However, adding co-surfactants to overcome the phase instability issue can compromise the ability of the surfactant formulation to reduce the oil/water IFT to ultralow values for effective oil mobilization and therefore, oil recovery. The objective of this study was to identify appropriate co-surfactants that can help overcome the aqueous instability of alkyl propoxylate sulfates at high temperature/high salinity conditions and maintain ultralow IFT for crude oils. A group of high mole ethoxylates of various structures was systematically investigated as co-surfactants in formulations with APS at temperatures up to 60 °C and salinities up to 22 % total dissolved solid containing divalents. The formulations that meet both aqueous stability and IFT reduction criteria were identified. The studied parameters are the co-surfactant structure and the surfactant/co-surfactant ratio. The static adsorption of the promising formulations on three types of sands (Berea, limestone and shale) was also evaluated. The finding of this study is advantageous in overcoming the challenges in EOR for HT/HS reservoirs.

Defoaming of Non-Aqueous Foams: Occurrence, Challenges and Silicon-free Defoamers Ramesh Varadaraj*[1], Ollie James[1], and George A. Smith[2],[1]*Sasol Performance Chemicals, USA;* [2]*Sasol North America, USA*

Abstract not available.

The Effect of Surface Roughness on Surfactant Adsorption at the Solid-Water Interface Brian P. Grady*,*University of Oklahoma, USA*

Surfactant adsorption from water onto a solid surface is important in applications such as laundry, hard-surface cleaning and enhanced oil recovery. For ~90% of the surfactant adsorbed, the driving force for adsorption is entropic, which in turn is a function of the adsorbed layer to exclude water. Our work shows that surface topological variations reduce adsorption, consistent with the expectation that such

variations reduce the ability of the adsorbed layers to pack well and exclude water. Through the use of a model surface, namely pillars with varying dimensions, we are able to show that topological variations can affect adsorption when the variations are on the order of tens of nanometers removed from the adsorbing surfactant.

Solvents and Surfactants for Cleaning Applications in Oil and Gas Jorge M. Fernandez, and Cornell Stanciu*, *Sasol North America, USA*

The choice of surfactants or surfactant-solvent blends proves to be critical in successfully solving various challenges the Oilfield industry is facing. Further complications arise from the ever-changing parameters that need to be accounted for, such as different crude oil compositions, different additives, compatibility issues of treatment formulations, chemical and geological differences between the rocks in different reservoirs, etc. This paper presents some case studies involving cleaning formulations developed by authors in the recent years in applications ranging from drill cuttings cleaning, to asphalt or bitumen cleaning off metal surfaces. The challenges between fine tuning the applied science knowledge and economic viability of a solution on industrial scale will also be discussed.

Cleaning Efficiency of soap Spent Bleaching clay and Palm Fatty acid Distillate Daniel Pioch[1], and Teerasak Punvichai*[2],[1]*CIRAD, UR 114 Biowooeb, TA-B 114/16, France;* [2]*Prince of Songkla University, Thailand*

This study deals with the co-valorization of spent bleaching clay (SBC) and palm fatty acid distillate (PFAD) –by-products of palm oil refining plants- through soap manufacture. When mixing SBC and PFAD (ratio 1:3), the reaction completion (92.5%) is surprisingly higher than expected, indicating a synergistic effect on the course of the saponification reaction. The water is also a critical parameter, 30% w/w of added water allowing the highest yield. When testing for cleaning efficiency the products having the highest soap content, those from individual by-products give a low microbial count reduction after hand-washing (30-37%). But a much better score (74%) is obtained when using SBC:PFAD soap mixtures. This improvement could be due to abrasive and absorption effects of the clay, combined to the high soap content. The acceptability through a panel test is good for all soaps when formulated with citrus oil. The most active product corresponds to a SBC:PFAD ratio close to the production one in refining plants. Therefore these results provide an easy way for co-valorising these by-products, after further optimizing the saponification reaction in this complex triphasic medium (aqueous solution, oil, clay).

Controlling the Physical Properties of Softener in a Continuous Manufacturing Process Fumiya Yamagishi*, Tatsuo Nagano, and Taku Nishio, *Lion Corporation, Japan*

Diversification of consumer needs based on recent lifestyle changes is altering the softener market structure. Consumers not only want more particular types of softness, the conventional function, but also lifestyle-accommodating functions such as fragrance and hygiene, resulting in a diversity of product variants. Efficiently producing a wide range of functions to meet these market needs is not only a matter of the formula; the manufacturing process also plays a major role. Adding ingredients with different physicochemical properties corresponding to this diversification of functions affects product qualities such as viscosity, homogeneity and stability as well as consumer usability. Therefore, we researched how to control these physical properties in the manufacturing process, specifically the continuous manufacturing process of liquid

crystal phase inversion emulsification, in which liquid crystals containing cationic surfactant are formed and then dispersed. We were able to establish a technique to ensure stable product viscosity and homogeneity by controlling conditions such as stirring and water content during liquid crystal formation according to the physical properties of the ingredients. This makes it possible to efficiently produce a variety of formulas, for example various fragrances and functional ingredients as well as microcapsules containing them, within the same manufacturing process.

The Role of Meso-structure of Citrus Pectin for its Emulsifying Performance Shaojie Zhao[1], Guifang Tian*, David Julian McClements[2], Hang Xiao[3], and Jinkai Zheng[1],[1]*Institute of Food Science and Technology, Chinese Academy of Agricultural Sciences;* [2]*Department of Food Science, University of Massachusetts Amherst;* [3]*Department of Food Science and Technology, University of Massachusetts, Amherst, USA*

There is a growing interest in using pectin as an emulsifier to deliver functional ingredients due to its natural source and good emulsifying capacity. Citrus pectin molecules assemble to aggregates in solution under multi-intermolecular interactions, and the meso-structure was important for the emulsifying performance. However, little information was known about the relationship between citrus pectin meso-structure parameter and its emulsifying performance. Herein, the meso-structure of citrus pectin was modulated by reducing molecular weight (hydrolysis for 0-240 min) and changing environmental condition (pH 2-7 and 0-100 mM NaCl). The meso-structure of citrus pectin and the various interfacial capacities were determined to illustrate the relationship between meso-structure and the emulsifying performance. Compared with the initial one, the aggregates of low molecular weight citrus pectin, obtained by hydrolysis, presented smaller size (from 1600 nm to 750 nm) and better interfacial ability (interfacial tension reduction 1 mN/m more), but the emulsifying performance became poorer with the reduction of molecular weight. In contrast, decreasing pH and increasing ionic strength not only reduced aggregate size and improved the interfacial ability, but also promoted emulsifying performance. From the SEM, it was found that acid and ionic strength resulted in compact meso-structure of citrus pectin in solution and at the interface, which brought about compact interfacial layer resisting coalescence of emulsion droplets during homogenization. In summary, the compact meso-structure of citrus pectin was vital for its emulsifying performance. The results provided a better understanding of the meso-structure, which may facilitate the utilization of citrus pectin as emulsifier.

S&D 3: Trends in Household Cleaning

Chairs: Mark Sivik, Procter & Gamble Co., USA; and Brian Sansoni, American Cleaning Institute, USA

Evolving Trends and their Influence on the Design of Fabric, Air and Home Care Products Mary B. Johnson*, *P&G Fabric and Air Care, USA*

Much of the world relies on commercially manufactured products for their laundry, indoor air management, and home cleaning needs. To ensure that these products continue to provide meaningful benefits it is crucial to understand the latest trends that influence consumer needs and challenges. This presentation uniquely combines decades of consumer research with a detailed analysis of evolving trends in consumer lifestyles, occupations, and habits and practices, textile fiber and hard surface composition, and advances in consumer appliance technology. The surprising conclusion of our analysis is that today's consumers face substantially more sophisticated and multi-facetted cleaning challenges than they did 10 or more years ago.

Commercialization Opportunities for Printed, Flexible, Stretchable and Functional Fabric Sensors and IoT. What does it mean to have a functional fabric? Eric Spackey*, *Advanced Functional Fabrics of America, USA*

Abstract not available.

Promoting Fragrance's Ability to Enhance Lives — People, Perfume & the Planet Farah K. Ahmed[1], and Lia K. Dangelico*[2],[1]*Fragrance Creators Association, USA;* [2]*Fragrance Creators Association, United States*

In addition to increasing enjoyment of everyday tasks, such as laundry and dishes, fragrance and scent often play a vital role in our fondest memories, emotions, and connections. This session will illuminate fragrance and the fragrance industry, including how Fragrance Creators Association is translating the story of fragrance for diverse audiences, educating on how fragrances are regulated, and advocating for sound science, innovation, and more. Attendees will come away with a better understanding of the power of fragrance beyond its ability to enhance lives.

Green Chemistry and Noncovalent Derivatization in Fabrics and Home Care Products John C. Warner*, *Warner Babcock Institute for Green Chemistry, USA*

The defining text "Green Chemistry: Theory and Practice" and the 12 principles of Green Chemistry were published twenty years ago in 1998 by John Warner and Paul Anastas. There are now dozens of Green Chemistry textbooks, journals, conferences, university courses and degree programs around the world documenting molecular level mechanistic approaches to reducing or eliminating negative impacts of materials and products on human health and the environment. In the early days of Green Chemistry, Warner, as an industrial chemist, develop the concepts of Noncovalent Derivatization, a first-principles approach to designing multimolecular complexes to control chemical and physical properties. In 2014 he received the Perkin Medal (consider the highest honor in US Industrial Chemistry) for this work. This presentation will discuss Warner's basic concepts of Green Chemistry and Noncovalent Derivatization. Examples of technologies developed and commercialized at the Warner Babcock Institute for Green Chemistry will be presented with an emphasis on approaches that are most relevant to fabric and home care products.

Product Manufacturers Approach to Ingredient Transparency and Sustainability Nancy Falk*, *Clorox, USA*

Clorox is a pioneer in ingredient transparency. Ten years ago, we pioneered online ingredient disclosure in cleaning products with Ingredients Inside. With

deadlines approaching for the New York and California ingredient disclosure legislation requirements, this presentation will talk about Clorox's efforts has effort to take ingredient transparency to the next level for both nonregistered and registered cleaning products, including the implementation of a fully integrated data system to aid in ingredient selection and disclosure and partnering with suppliers for accurate raw material compositions.

Biomaterials and the Circular Economy Michael A. Saltzberg*, *DuPont Industrial Biosciences, USA*

One of the most important trends in household cleaning is the demand by consumers and governments around the world to reduce the environmental impact of products, packaging and processes. Over the past few years, this thinking has evolved to include all aspects of a product's life cycle, from the raw materials that go into a product, to its manufacturing process, to how it is used by consumers, and finally to what happens to the product when its useful life is over. As described by the Ellen MacArthur Foundation, the ideal system is a Circular Economy where waste and depletion of finite resources at all stages of the product lifecycle are minimized by slowing, closing, and narrowing energy and material loops during the design of new products. Biomaterials, that is materials made from renewable rather than fossil-based resources, can play an important role in moving towards this ideal state. This talk will give an innovator's perspective on specific examples of success stories as well as some of the challenges that remain for Biomaterials.

Appliance Manufacturers Trends and Approach to Sustainability Brigitte Mader-Urschel*, *GE Appliances, USA*

This session explores sustainability trends for major appliances products. Consumer trends call for deeper definition of materiality in the appliances industry, to go beyond regulatory drivers to an expanded view of environmental and human impact. This session will review the materiality in the appliances sector, and how consumer trends and behavior patterns on components and detergent selection, lifecycle assessment and other areas can drive changes in environmental footprint and result in a broader view of impact as manufacturer.

S&D 3.1: General Surfactants II: Surfactant Synthesis and Fundamental Properties
Chairs: George A. Smith, Sasol, USA; and Sanja Natali, ExxonMobil Chemical, USA

An Analytically Defined Fire-sppressing Foam Formulation for Evaluation of Fluorosurfactant Replacement Katherine M. Hinnant[1], Spencer L. Giles[1], Arthur W. Snow*[1], John P. Farley[1], James W. Fleming[2], and Ramagopal Ananth[1],[1]*U.S. Naval Research Laboratory, USA;* [2]*NOVA Scientific Inc., USA*

A 4-component, analytically defined, reference fluorosurfactant formulation (Ref-aqueous film forming foam [AFFF]) composed of 0.3% fluorocarbon-surfactant concentrate, 0.2% hydrocarbon-surfactant concentrate, and 0.5% diethylene glycol mono butyl ether by volume in distilled water was found to have rapid fire extinction comparable to a commercial AFFF in tests conducted on a bench scale and a large scale (28 ft^2, part of US Military Specification, MILF-24385F). The Ref-AFFF was analytically characterized to provide the identity and quantity of the chemical structures of the surfactant molecules that were lacking for commercial AFFF formulations. To arrive at an acceptable Ref-AFFF formulation, three candidate formulations containing different hydrocarbon surfactants in varying amounts were evaluated and ranked relative to a commercial AFFF using a bench-scale fire-extinction apparatus; varying the hydrocarbon surfactant was found to affect the fire-extinction time. The ranking was confirmed by the large-scale tests suggesting that the bench-scale apparatus is a reasonable research tool for identifying surfactants likely to succeed in large-scale testing. In the future, replacing the fluorocarbon surfactant with an alternative surfactant in the Ref-AFFF enables a direct comparison of fire extinction and environmental impact to identify an acceptable fluorine-free formulation. This Ref-AFFF also serves as a starting point design and preparation of new surfactants for such fluorine-free and environmentally acceptable formulations.

Correlation Between Hydrophilic-Lipophilic Deviation (HLD) and Detergency of Different Oily Soils Parichat Phaodee*, and David A. Sabatini, *University of Oklahoma, USA*

In this work, detergency of oily soils with different equivalent alkane carbon number (EACN) was carried out to correlate detergency with HLD values. Different EACN oil mixtures were evaluated in detergency studies using C10-4PO-SO4Na with different salinities (low to high salt levels). The surfactant salt scans were able to produce microemulsions Type I, Type III and Type II regions at washing temperature of 25C for all the oil systems studied. Then, the salinity scan values were converted to HLD values using the constructed HLD equation which was obtained via middle microemulsion formulations of different known EACN oils. The HLD parameters of C10-4PO-SO4Na surfactant were determined to be as follows: surfactant head group (k) of 0.053 and a surfactant characteristic curvature (Cc) of -2.29. The detergency results of different EACN oil mixtures showed that good detergency for all oils studied was observed at different optimal salinities depending on the EACN of oils. Finally, the correlation between HLD (conversion of salinity to HLD) and detergency demonstrated highest detergency for HLD values in the range of -3.00 to 0.00 for all oil systems. This trend demonstrates that good detergency corresponded with the microemulsions between Type I and optimum Type III (S*) which exhibited a favorable region with the interfacial tensions (IFTs) well below 1 mN/m. Thus, while the optimal salinities varied widely for the different oil systems, the results converged to common values of HLD, highlighting the utility of using the HLD approach in design surfactant formulations for detergency.

Tuning Structuring in Aqueous Media via Surfactant-polymer Interactions Paschalis Alexandridis* and Marina Tsianou, *University of Buffalo, SUNY, USA*

Mixtures of surfactants and polymers afford great flexibility in conferring structure and function in waterborne formulations applied to coatings, home and personal care products, food and drinks, pharmaceutics, and enhanced oil recovery. Underlying such structure and function are inter- and intra-molecular interactions that depend on the (i) polymer chemistry, architecture and concentration, (ii) surfactant type and concentration, (iii) solvent conditions (e.g., pH, ionic strength, presence of cosolvents or cosolutes), (iv) interfaces and surfaces (e.g., presence of colloidal particles), and (v) external stimuli (e.g., temperature, shear). The presentation will highlight examples from our research on the formation and structure of complexes by commercially available anionic surfactants and nonionic poly(ethylene oxide)-based polymers in water, as affected by the ability of the polymer to associate upon incorporation of hydrophobic poly(propylene oxide) segments, the hydrophobicity of the surfactant (aliphatic hydrocarbon vs fluorocarbon chain), and the hydrophobicity of the solvent (added ethanol, salt or ionic liquids).

Characteristic Curvature of Secondary Alcohol Ethoxylates and Emulsion Stability Michael Tate*[1], Daniel Miller[2], Emily Bellairs[1], Bethany Karl[1], and Christopher J. Tucker[1], *[1]The Dow Chemical Company, USA; [2]Dow Chemical Company, USA*

Secondary alcohol ethoxylates enable performance driven differentiation across multiple applications from cleaning and oilfields to agrichemicals. Here we study the impact of changes to the structure of secondary alcohol ethoxylates on the formation and stability of emulsions, including variation of the EO length from 5 to >20. We then compare the properties of formulations to existing theories, including hydrophile-lipophile deviation (HLD), to elucidate structure/performance relationships for emulsion and microemulsion directed applications. These relationships are then validated through experiments using high throughput experimentation techniques to formulate, measure, and analyze emulsion phase behavior at varying temperatures and surfactant, oil, and salt type and concentration. This approach combines three specific tools: 1) a multichannel liquid handler, 2) a custom-built image-capture station that captures images under well-controlled, uniform lighting conditions, and 3) a custom data-analysis algorithm to identify and determine the volumes of each phase. Overall, the results presented here will enable rapid formulation of emulsions for each of the above mentioned applications.

Effect of Alkyl Chain and Oligomer Distribution on Performance of Ziegler Alcohol Ethoxylates Tamra Weemes*[1], and George A. Smith[2], *[1]Sasol Performance Chemicals, USA; [2]Sasol North America, USA*

The effect of alkyl chain length and oligomer distribution of nonionic surfactants on physiochemical and performance properties has been investigated. The effect of peaking the oligomer distribution on micellization was determined by equilibrium and dynamic surface tension measurements. Pendant drop and drop volume measurements were used to measure the interfacial tension against different types of oils. The effect of narrow range oligomer distribution on performance was determined by rheology, foam measurements and detergency in laundry and hard surface cleaning applications. Peaking the oligomer distribution increases the critical micelle concentration (CMC) and the surface tension at the CMC by reducing the amount of unreacted alcohol and

low mole ethoxylates. Peaking the distribution also increases the rate at which the surfactant diffuses from the bulk solution to the interface. Narrow range ethoxylates show lower interfacial tension against polar and nonpolar oils. This increases the solubilization capacity of the surfactant and improves cleaning properties in laundry and hard surface applications.

The Effect of Surfactant Systems, Alcohol Types and Salinity on Cold Water Detergency of Triglyceride Semisolid Soil Parichat Phaodee*, and David A. Sabatini, *University of Oklahoma, USA*

In previous work, the detergency results showed that 0.1 w/v% C14-15-8PO-SO4Na with 100% branching /90 mM 1-octanol/4%NaCl (the previous best surfactant formulation) removed semisolid coconut oil as high as 95.4±0.2% at 10C corresponding to lower interfacial tension (IFT) and contact angle. The present work attempts to further investigate the effect of different anionic extended surfactant systems and branching octanols on cold water detergency of solid coconut oil at washing temperature of 10C. In this work, three more anionic extended surfactants were studied; 50% branching LC14-15-8PO-SO4Na, 50% branching LC14-15-8PO-3EO-SO4Na and 50% branching LC14-15-8PO-7EO-SO4Na. The detergency results of all 50% branching anionic surfactants did not improve upon the 100% branching C14-15-8PO-SO4Na; this could be attributed to higher minimum IFTs. Furthermore, 2-octanol and 2-ethyl-hexanol were selected as branching octanols to further study the effect of branching alcohol on detergency. Interestingly, detergency with 0.1 w/v% C14-15-8PO-SO4Na/90 mM 2-octanol/2%NaCl (an optimum surfactant formulation) was 98.3±2.4% removal which was comparable to the previous best detergency formulation. The detergency results showed that detergency correlated with lower contact angle reflecting higher wettability. It also showed that only surfactant formulations with added octanols and S* revealed a promising solubilization result, and that in these systems the solid coconut oil was softened by surfactant/octanols penetration. This insight showed that good cold water detergency could be attributed to semisolid soil-softening process required as a preparing semisolid soil removal step which allowed surfactant/octanols to wet the semisolid soil easier resulting in increasing solubility and also wettability.

On the Oil-like and Surfactant-like Characterization of Polar Oils Edgar Acosta*, and Amir Ghayour, *University of Toronto, Canada*

Polar oils such as long chain alcohols and fatty acids are quite relevant in detergency, the alcohols present as the unreacted fraction in alcohol ethoxylates, the fatty acids present as a fraction of cooked oils. Alcohols, esters and ethers are also present in formulations as fragrances. Their polarity gives them a surfactant-like behavior along with their oil-like behavior. This presentation describes an approach that introduce both of these characteristics within the hydrophilic-lipophilic difference (HLD) framework. The surfactant-like segregation of the polar oils to the oil-water interface is accounted for using a Langmuir-type model. The proposed framework can account for changes in formulation conditions as a function of the polar oil concentration. The implication of the findings for detergent and hard surface cleaning formulations will be discussed.

Characteristic Curvature of Various Commercial Laundry Formulations Jeff Harwell, Brian P. Grady, and Michael T. Warren* *University of Oklahoma, USA*

The hydrophilic-lipophilic difference (HLD) equation is a semi-empirical equation that was originally developed to correlate the formation

of microemulsions with surfactant characteristics, oil characteristics etc. Even though the surfactant concentration is not sufficient in a typical washing machine to form a microemulsion, recent work in this area suggests that cleaning of liquid and solid triglycerides is maximized when HLD is near zero. One obvious question from this work is what is the value of the parameter that quantifies the surfactant characteristics in the HLD equation in a specific commercial laundry detergent. This parameter, called the characteristic curvature (Cc), is somewhat analogous to the HLB number. For a hydrophilic surfactant, Cc is less than zero while for a hydrophobic surfactant, Cc is greater than zero. This work was motivated by an unfounded belief that the Cc of all commercial detergents would be approximately the same. Normally the measurement of Cc requires thermodynamic equilibrium; however, with commercial detergents the existence of kinetic barriers typically does not allow equilibrium. Instead, we are using minimum coalescence time to determine Cc; the method will be detailed in the talk. Results for 7 different detergents with varying manufacturers and price points indicate that all but one detergent varies in Cc between -1.35 to -1.9, which we consider to be a narrow range. We plan to measure a total of 15-20 different commercial detergents, and all results will be presented.

New Sugar-based Surfactant Compositions

Phillip K. Vinson* and Ryan M. West, *The Procter & Gamble Co., USA*

Novel surfactants based on sugar amides or sugar amines have been synthesized and studied. Improved physical properties will be discussed based on both the surfactant hydrophobe, e.g., from new sources of unique methyl esters, as well as from mixtures of the sugar-based head group.

BIO 4.1 / S&D 4: Biosurfactants and Environmentally Friendly Ingredients
Chairs: Sujan Singh, Arkema, USA; and Douglas Hayes, University of Tennessee, USA

Comparative Antimicrobial Efficiency Among C18 and C22 Sophorolipid Congeners towards Select Gram+ Bacterial Strains Richard D. Ashby*, and Daniel K.Y Solaiman, *USDA, ARS, ERRC, USA*

Many microbial glycolipids are effective antimicrobial agents. Sophorolipids (SLs) are naturally composed of sophorose (a disaccharide) connected to a fatty acid 'tail' through a glycosidic bond and depending on the producing strain, the substrate, and the culture conditions, the structure of the lipid tail may vary in terms of chain length and number of olefinic groups. The antimicrobial activity of SL seems to be greater against Gram-positive (Gram+) bacteria. This presentation will focus on the antimicrobial efficiency of different SL congeners against select Gram+ bacterial strains including *Propionibacterium acnes*, various *Streptococci* and *Lactobacilli* strains commonly found in the oral cavity and *Listeria monocytogenes*, a strain associated with food-borne illness. This presentation will present our recent findings on the production and purification of C22 SL isoforms from *Pseudohyphozyma bogoriensis* and provide a comparative assessment of the antimicrobial efficiency for various SL congeners produced by both *Starmerella bombicola* and *P. bogoriensis*.

How Biosurfactants Can Enable Degreasing J. R. Bennett[1], Eric Theiner*[1], and Stephanie Hackney[2],[1]*Evonik Corporation, USA;* [2]*Evonik Corporation, United States*

Biosurfactants such as sophorolipids and rhamnolipids are gaining considerable interest because of their utility in forming emulsions as well as the potentially positive toxicity and environmental attributes. By combining these types of surfactants with environmentally preferable lipophilic materials one can take advantage of basic emulsion properties to show effective degreasing. This presentation will show the benefits of one approach in removing heavy industrial greases and the resulting formula options revealed.

The Combined Effects of Soap and Sophorolipids in the Development of Mild Body Wash for Sensitive Skin Glen Lelyn Quan*[1], Chie Matsubara[1], Yoshihiko Hirata[1], Satoshi Yoshida[1], Maiko Iwai[1], Shinji Hamaguchi[1], Etsuko Komiyama[2], and Shigaku Ikeda[1],[1]*Saraya Co., Ltd. , Japan;* [2]*Juntendo University, Japan*

Skin care is one of the cited pillars of treatment according to the Atopic Dermatitis Treatment Guidelines released by the Japanese Ministry of Health, Labor and Welfare. In order to control *Staphylococcus aureus* flora, the skin should be washed by showering, bathing, followed by topical treatment as necessary. However, routine washing can be harsh to the skin, making milder cleansing agents more desired. Sophorolipids are promising glycolipid biosurfactants which have known characteristics such as excellent detergency and good rinsability, to name a few. Another quality to explore is its low-irritating effect on the skin, making them suitable to be used in formulations for sensitive skin. We tried to incorporate sophorolipids in formulations with soap and other components to develop a mild body wash. After establishing a stable formulation, effects of sophorolipids in the formulation were observed through sensory tests and their effect on the stratum corneum barrier function, followed by safety evaluation and comparison with other commercial products. Furthermore, a clinical evaluation involving 200 patients of Juntendo University Hospital with various skin diseases (including those with atopic dermatitis) was also performed. The obtained data showed

improvement on the degree of skin dryness and skin itchiness of patients after two weeks of use. It can be concluded that the combined effect of soap and sophorolipids in the developed mild body wash provide cleansing action that is also safe and soothing, even for patients with sensitive skin.

Optimal Regulation of Oxygenation for Coordination of Rhamnolipid Productivities and Residual Fatty Acid Content in Fermentation of *Pseudomonas aeruginosa* Qin Meng*,*Zhejiang University, China*

Rhamnolipids are multipurpose surface-active molecules produced by the bacterium Pseudomonas aeruginosa. Despite the high reputation of biosurfactants, such as low toxicity, biodegradability and high stability, these compounds have not been widely used because of the high cost of production and the difficulty on purification. Vegetable oil is believed to be the best raw material for rhamnolipid fermentation. The rhamnolipid synthesis from oil prefer to a medium aeration, which provide an inhibition of the microaerobic denitrification. Nevertheless, the severe foaming become a big problem in aerobic rhamnolipid fermentation, decreasing the rhamnolipid yield. Meanwhile, the residual fatty acid with similar lipid tails as rhamnolipids usually exacerbate the difficulties on the final separation and purification which are critical for the bioprocess of biosurfactant detergent. Hence, dissolved oxygen concentration (DO) will be extremely important in coordination of foaming, denitrification and β-oxidation in biosynthesis of rhamnolipids by fermentation. This study will monitor the rhamnolipid productivity and residual fatty acid content using different oxygenation level which was represented by the oxygen transfer coefficient (KLa) as a result of agitation and aeration.

Aspartic Acid-based Ampholytic Amphiphiles: Synthesis, Characterization, and pH-Dependent Properties at Air/Water and Oil/Water Interface Weiwei Cheng[1], Sampson Anankanbil[2], Liu Guoqin[3], and Zheng Guo*[4],*[1]South China University of Technology, China; [2]Dept. of Engineering, Aarhus University, Denmark; [3]School of Food Science and Engineering, South China University of Technology, China; [4]Aarhus University, Denmark*

A facile and two-step strategy was employed to synthesize two series of novel aspartic acid-based ampholytic amphiphiles from sustainable and commercially viable substances as starting materials. The molecular structures of the synthetic compounds were well identified by MS and 1H/13C analysis, and the physicochemical, pH-dependent foaming and emulsifying properties were evaluated by the use of multiple techniques such as FTIR, DSC, Langmuir−Blodgett study, and fluorescence microscopy imaging. Due to the coexistence of amino and carboxyl groups in the synthetic compounds, the compounds presented varying charges (cationic, ampholytic, and anionic) depending on the pH of the medium compared to the dissociation constants (pKa). Compounds with cationic (pH 1.0) and anionic (pH 9.0) forms had significantly higher γ0.1 and CMC values than that with ampholytic forms (pH 7.0). Sn-1-lauroyl-sn-3-aspartic acid (compound 3) at neutral and alkaline conditions displayed comparable foaming properties including foaming, calcium-tolerance, and temperature-resistance ability with commercial sulfonate SDS, and thus might be a promising alternative to SDS, applied in personal care products and detergent formula. Sn-1-palmtoyl-sn-3-aspartic acid (Compound 5a) with ampholytic structure was proved as the most excellent stabilizer for the preparation of oil-in-water nanoemulsions compared with palmityl aspartic acid (compound 5b), commercial food ingredient DATEM, and

glyceride monopalmitate at aqueous phase pH 7.0. Thus, it has promising use as a pH-dependence emulsifying agent in various fields.

Antimicrobial Efficacy of Oxygen-Based Bleach Systems Sam Adamy*, *Church & Dwight Co. Inc., USA*

Systems which generate oxidative molecules in the form of a peroxide or a peracid are attractive for use in a number of applications, not only from the standpoint of stain removal, but for antimicrobial action as well. Such systems additionally exhibit favorable environmental and toxicity profiles, thus making them well-positioned for consumer and regulatory acceptance. For example, two components associated with oxygen-based bleaching, sodium percarbonate and tetraacetylethylenediamine (TAED), have been safely employed in the marketplace for many years, and produce relatively benign waste streams. Achievement of required efficacies for sanitization and/or disinfection claims can be challenging, however. In this presentation, examples of oxygen-based bleaching systems and associated efficacies in laundry and other home care applications will be presented, along with comments around the applicability to claims of disinfection and sanitization. Data will be presented on both antibacterial and antiviral outcomes.

Fatty Acid, Methyl Ester and Vegetable Oil Ethoxylates George A. Smith*, *Sasol North America, USA*

Soap is the first and oldest example of a biobased surfactant. Soap is prepared by saponifying fats and oils with caustic. Soap has been used for over 4500 years for personal cleaning and washing of clothes. In personal cleaning products, the high pH of soap can irritate the skin and eyes and soap also suffers from sensitivity to salinity and hard water ions. With the advent of modern industrial chemistry, the reliance on soap has declined. Fatty acid ethoxylates (FAE) are prepared by reacting fatty acids with ethylene oxide or polyethylene glycol (PEG). Both reactions produce a mixture of ethoxylated fatty acid, bis fatty acid ester and PEG. FAE can be used in neutral pH and is relatively insensitive to hard water ions but suffers from low yields due to the transesterification reaction. Methyl ester ethoxylates (MEE) were originally developed to improve the efficiency of fatty acid ethoxylates. Reacting fatty acid methyl ester with ethylene oxide using a calcium or magnesium based catalyst or esterification of fatty acids with polyethylene glycol methyl ether (MPEG) produces MEE high yeilds. MEE is soluble at neutral pH and shows favorable detergency but suffers from hydrolytic stability issue in alkaline solution and does not build viscosity in low active formulations through the salt effect. Vegetable oil ethoxylates (VOE) are made by direct ethoxylation of triglycerides or transesterficiation of tryglycerides with ethoxylate glycerin. VOE show good surface activity and are exceptionally mild to skin and eyes. VOE is used primarily in personal care as emollients and foam boosters in rinse off products.

Biobased Surfactants: An Overview Douglas G. Hayes*, *University of Tennessee, USA*

Biobased surfactants continue to gain increased attention and employment, despite the relatively low cost of fossil fuels in today's world. In this paper, I will provide a review of biobased surfactants, providing information on underlying trends relating to biobased surfactants, particularly in terms of environmental sustainability, and describe new and emerging biobased surfactants.

Laundry Sustainability vs. Laundry Sanitization: The Tension and the Solutions Nancy Falk*,*Clorox, USA*

Most of the laundry process carbon

footprint is related to the energy required to heat the wash water. As a result, wash temperatures have decreased, chemistries have become less harsh, and cloth-to-wash water ratios have increased. Studies have also shown that microbial contamination in laundry is common and spreads readily within and between washloads, exposing consumers to pathogens. In this talk, innovations in laundry to advance sustainability are contrasted with microbial contamination, and current chemical solutions are reviewed.

Biodegradable Dispersants for Phosphate Free Automatic Dishwashing Detergents Scott A. Backer*[1], Severine S. Ferrieux[2], Eric P. Wasserman[1], Paul P. Mercando[1], Randara Pulukkody[1], Anurima Singh[1], Lin Wang, Ken Laughlin[4], Steve Arturo[1], and Lu Bai[1], *[1]Dow Chemical Company, USA; [2]The Dow Chemical Company, France*

Over the last decade, a significant shift in the sustainability profile for detergent formulations has been taking place. In order to combat eutrophication of waterways, regulations requiring the removal of sodium tripolyphosphate from detergents in the developing world have been proposed and implemented. This has radically altered the strategies of formulators, as new combinations of ingredients are required to take the place of once-abundant phosphates. One area of research has been on novel polymers capable of dispersing inorganic salts formed as detergents come into contact with hard water. These dispersants, classically low to moderate molecular weight polyacrylic acids, are excellent performers which demonstrate only minimal biodegradability. This talk will discuss strategies used to design and test a new class of biodegradable dispersants which exceed the performance of current dispersants while significantly increasing the overall level of biodegradable polymeric carbon.

Greener and Milder Functionalized Sugar-Based Surfactants for Home Care and Industrial Applications Robert J. Coots*, Dennis Abbeduto, and Andy Sun,*Colonial Chemical, USA*

Colonial Chemical Inc. is a leading supplier of naturally-derived, functionalized sugar-based surfactants with the trade names of Suga® and Poly Suga®. These products meet the growing demands in Household and Personal Care industries to replace ingredients which have Prop 65 concerns or are highly irritative, such as alcohol alkoxylates and sulfates. Suga®Nate is a series of 100% naturally-derived anionic polyglucoside surfactants, produced using concepts well known in the field of green chemistry, as opposed to the traditional means for manufacturing sulfates and sulfonates. These ingredients are qualified for Safer Choice Direct Release and they show no, or very low irritation to eyes and skin. These surfactants show good detergency and foaming and have unique attributes to applications in home, pet, and vehicle care applications. Suga®Fax D10NC is a 100% natural, green hydrotrope with improved performance versus Sodium Xylene Sulfonate (SXS). This product can be used at lower levels with improved performance while avoiding the toxic impurities in SXS, which are of Prop 65 concern. Poly Suga®Mulse products represent 100% biobased, EO-free emulsifiers for fragrances and other emulsion formulations. The nonionic surfactants function much like ethoxylated fatty alcohols, with superior performance and without the concern of residual EO or 1,4-Dioxane. Poly Suga®Quat surfactants, with their cationic nature, have been shown to boost cleaning of greasy soils, and have the ability to boost the efficacy of a preserved formulation.

S&D-P: Surfactants and Detergents Poster Session
Chair: Mike Wint Amway Corp., USA

1. **Amide Types of Gemini Surfactants Derived from Diethyl Tartrate.** Daisuke Ono*, Keisuke Yoshida, Yuki Morimoto, Shintaro Kawano, Hirofumi Sato, Motohiro Shizuma, and Araki Masuyama, *Osaka Research Institute of Industrial Science and Technology, Japan*

The development of surfactants with excellent surface-active properties or additional functions has become desired. Therefore, it has come to be interest to develop "gemini" surfactants which are synthesized by connection of the traditional monomeric amphipihilic molecules with a spacer. They have a high performance such as good water solubility, excellent micelle-forming property and high ability to lower surface tension. Low molecular-weight gelator is also attractive materials. In this work, amide types of gemini surfactants were prepared by a reaction of diethyl tartrate with long chain amine, and subsequent sulfation without any expensive reagents and special equipment. We discussed about their surface-active properties and gel-forming properties in various solutions. The viscosity of the toluene solution containing the surfactant were higher than blank solvents.

2. **Assessment of Skin Mildness of Personal Care Cleansers.** Brajesh Jha*[1], Aixing Fan[1], Hongwei Shen[1], Derek Kim[2], Irina Chernyshova[2], Ponisseril Somasundaran[2], and Parta Patra[2], *[1]Colgate Palmolive Co., USA; [2]Dept. of Earth and Environmental Engineering, Columbia University, USA*

For personal care cleansing products, the nature of the skin-surfactant interactions determines the mildness of the product. To study the mildness of four personal care cleansers, we assessed the skin-surfactant interactions by determining the water retention capability of the skin using two techniques. In one of the techniques, water retention was measured through collagen swelling. In the other complementary method, the water retention of the pig skin* was assessed with a Raman spectroscopy technique. In the study, pig skin samples were subjected to D2O and formulation mixture. The Raman spectral peaks representing D2O were accounted for estimating the water retention capability of the skin. In addition, Critical Micelle Concentration (CMC) curves were measured for these formulations to gain fundamental insights on their performance. All three methods resulted in a consistent ranking of the product mildness.
* pig skin was sourced from the food chain

3. **Monoglyceride-stabilized Pickering Emulsions as Vehicles for Controlled Release.** Malek El-Aooiti*, Auke de Vries, and Dérick Rousseau, *Ryerson University, Canada*

Water-in-oil emulsions (W/O) can be stabilized by interfacially adsorbed glycerol monostearate (GMS) crystals. This is achieved by melting the GMS wax in the oil phase of the emulsion followed by shear-cooling to induce crystallization of interfacially adsorbed GMS. Emulsions formulated using this method have shown to be robust, stable during storage, and can encapsulate aqueous material with high efficiency. Previous efforts from our group demonstrated that W/O emulsions with interfacially bound glycerol monostearate (GMS) crystals can be destabilized by the addition of a secondary surfactant. Addition of the surfactant, sorbitan monooleate (SMO), subsequently resulted in destabilization of emulsion droplets followed by release of aqueous cargo. In the current study, it was found using microscopy, that droplets undergo rapid coalescence and decomposition upon exposure to SMO. The current study explores

this phenomenon at different length scales. Light and fluorescence microscopy were used to study the effect of added surfactant on emulsion microstructure and droplet morphology, while dynamic contact angle studies were used to determine the effect of SMO on the wetting behaviour of the GMS crystals. This works aims to elucidate a mechanism of action by which added surfactant destabilizes monoglyceride-stabilized W/O Pickering emulsions to design tuneable controlled release systems.

4. **Nanoparticles Stabilized Foams for Enhanced Oil Recovery using Carboxylate-based Extended Surfactants.** Pattamas Rattanaudom*[1], Ben Shiau[2], Ampira Chareonsaeng[1], and Uthaiporn Suriyapraphadilok[1], *[1]The Petroleum and Petrochemical College, Chulalongkorn University, Thailand; [2]University of Oklahoma, USA*

The adding of nanoparticles in a surfactant-stabilized foam system shows remarkably potential to improve the foam stability. Recently, the novel carboxylate extended surfactants show several benefits regarding foam stability, solubility, thermal stability in harsh conditions. Notwithstanding, the behaviors foam prepared by novel carboxylate extended surfactants as a foaming agent is significantly influenced by pH values. In this work, the carboxylate-based extended surfactants, fatty alcohol ethoxylated carboxymethylated (SOLOTERRA@ 172) at the controlled pH (pH9) in the presence of SiO2 nanoparticles is conducted as a foam system. The effect of the nanoparticles-surfactant foam is investigated on the foam behavior in the sand pack column at controlled temperature (60˚c) and in the presence of API brine. The efficiency of oil recovery in the porous media is evaluated at different temperatures and brine conditions. In addition, the improvement in oil recovery at different nanoparticles concentrations also is evaluated and compared. The crude oil composition at each pore volume is investigated by a high-performance liquid chromatography (HPLC). Thus, the selection of suitable design condition of carboxylate-based extended surfactant/nanoparticles foam system in enhanced oil recovery process will be discussed.

5. **DSC and 3D X-Ray Microscopy Study on Bar Soap Structures.** Aradhana Das and Hongwei Shen*, *Colgate Palmolive, USA*

The structure of bar soaps is critical to the consumer experience. Thus, understanding the structures of bar soaps is paramount for producing the best products with nice lather, minimal cracking, and the right hand feel along with other attributes since both formulation and process can impact these structures. Historically, differential scanning calorimeter (DSC) & X-Ray Diffraction (XRD) (Gupta, JAOCS, 1991) were reported for identification of delta, beta, and omega soap phases and then related to lather properties for pure fatty acid based soaps. In the current study, we focus on the study of bar soaps with additives such as calcium carbonate and/or starch. DSC is used for soap structure analysis. It is found that the previously identified soap structures such as delta, beta, and omega were not influenced by these additives. The composition of the structures also directionally correlates to the performance such as lather properties, based on expert panel results. In addition, we applied a new technique, 3D X-ray microscopy, to understand the distribution & dispersion of additives in the soap matrix. It is found that processing can impact the dispersion and sometimes cause agglomeration of additives in bar soap. It is learned that 3D X-ray microscopy can be a powerful tool to study the distribution and agglomeration of additives during the soap making processes