2020 AOCS Annual Meeting & Expo Surfactants and Detergents Abstracts

June 29 to July 3, 2020

Hosted online by the American Oil Chemists' Society (AOCS)

For more information, please visit https://annualmeeting.aocs.org.

Surfactants and Detergents

Monday, June 29, 2020

Session Time: 8:25 AM - 10:10 AM

Presentation Time: 8:25 AM - 8:30 AM

Track: Surfactants and Detergents

Introduction: HLD/NAC

Co-Chair: Edgar J. Acosta - University of Toronto
Co-Chair: Sanja Natali, PhD - ExxonMobil Chemical

The hydrophilic lipophilic deviation (HLD) and the net-average curvature (NAC) are becoming common tools in the arsenal of the surfactant formulator. These sessions will include invited talks from industry and academia presenting an introductory overview of these concepts and their application in a wide range of fields, including, oilfield chemistry, agrochemical, cleaning, detergents, cosmetics and pharmaceutical formulations.

Monday, June 29, 2020
Session Time: 8:25 AM - 10:10 AM

Presentation Time: 8:30 AM - 8:30 AM

Track: Surfactants and Detergents

(3761) Using HLD to Find Solutions, Without Knowing Your Parameters

Presenting Author: Matthew Lyon, MBA - BASF

A production site had an issue with high TOC content in their wastewater stream. This translated into over $5 million spent each year in disposal costs. The contaminant was a mixture of ethoxylated surfactants and polyethylene glycol at 10% total solids. The plant wanted a cost effective method to clean the waste water. The problem was two-fold, finding a method to

remove both surfactant and the dissolved polymer. As the Cc values were not known of the mixture, best guesses inferring negative values were used. Hansen Solubility was used to identify the top solvent extraction candidates. Dichloromethane was identified as having similar HSP values. It also had the benefit of having a -14 EACN value. This would push most ordinary surfactants into +HLD territory, resulting in both surfactant (w/o emulsion) and PEG dissolved in the oil phase. This would then be allowed to phase separate for easy removal of contaminant. The results were confirmed through use of Salager diagrams to verify +HLD, and LOD test to confirm the extraction of both surfactant and polymer. All surfactant was removed in the first wash, with 1% remaining polymer to be removed in the second, smaller extraction. Without knowing our Cc values of the surfactant, we solved the problem by using the HLD framework to shift the system to a w/o emulsion through choice of oil. The oil was further able to extract the polymer with its similar HSP values.

Monday, June 29, 2020
Session Time: 8:25 AM - 10:10 AM

Presentation Time: 8:55 AM - 9:20 AM

Track: Surfactants and Detergents

(3817) Accounting for Concentration Effects in the Application of Hld Modeling to Nonionic Surfactants

Presenting Author: Gregory P. Dado, PhD - Stepan Company

Nonionic surfactant concentration can have a large impact on the temperature-dependent behavior of Surfactant-Oil-Water (SOW) systems. One of the limitations of commonly reported Hydrophilic-Lipophilic Deviation (HLD) modeling approaches is the lack of accounting for this concentration dependency. In this paper, quantitative relationships between alcohol ethoxylate concentration and SOW phase inversion temperature (PIT) will be reported in the context of HLD model parameterization. Dynamic temperature scan methods will be described that enable facile determination of PIT vs. surfactant concentration functions. Conversion of PIT data into to HLD parameter functions will also be described, together with the application of resulting HLD models to practical formulation problem solving such as oil solubilization and emulsion stability optimization.

Monday, June 29, 2020
Session Time: 8:25 AM - 10:10 AM

Presentation Time: 9:20 AM - 9:45 AM

Track: Surfactants and Detergents

(3866) Hard Surface Cleaner Development with HLD-NAC Principles

Presenting Author: Eric R. Theiner, MS - Evonik Industries

It is well known that adopting the Hydrophilic-Lipophilic Difference and Net Average Curvature (HLD-NAC) models provide opportunities for easily predicting oil/water systems with minimal interfacial tension between phases. It has also been demonstrated how minimal interfacial tension leads to effective cleaning systems when the soil is well defined. Two additional parameters that also impact cleaning are substrate wetting and surfactant monomer diffusion to the cleaning solution/soil interface. This discussion focuses on how utilization of the concepts behind HLD-NAC can be combined with the latter two to provide an efficient and effective hard surface cleaner.

Tuesday, June 30, 2020
Session Time: 11:45 AM - 1:00 PM

Presentation Time: 12:10 PM - 12:10 PM

Track: Surfactants and Detergents

(3888) Malodor Reduction from Cloth via Fragranced Microcapsules in Liquid Detergent

Presenting Author: Tamara Hopkins - IFF

Objective/Hypothesis: To demonstrate malodor reduction through fragrance design and physical malodor removal from the headspace using fragranced microcapsules in detergent. Methods Used: Sensory panels and instrumental headspace analysis. We developed sensory protocols for testing the complete malodor control technology solution in detergent vs. synthetic malodor & real malodor. Malodor reduction was demonstrated through relevant in use examples and analytical methods were utilized to show physical reduction of malodor. The topic of capsule suspension will also be covered as this is a challenge for liquid detergents. Results: We obtained consumer perceivable malodor reduction in relevant real world applications with the product containing the fragrance microcapsules vs. product without the technology. The consumer perceivable benefit is also paired with instrumental headspace data, therefore proving physical malodor removal with technology. We were also successful with suspending capsules in a liquid detergent application in order to deliver the technology in this particular laundry application/. Conclusions: Fragranced microcapsules are effective at reducing malodor in a laundry detergent and demonstrated in a real world application.

Tuesday, June 30, 2020
Session Time: 11:45 AM - 1:00 PM

Presentation Time: 12:35 PM - 1:00 PM

Track: Surfactants and Detergents

(3478) Correlation Between Detergency of Different Oily and Solid Non-Particulate Soils and Hydrophilic-Lipophilic Deviation (HLD)

Presenting Author: Parichat Phaodee, PhD - University of Oklahoma

This research examined the correlation between the detergency of soils with varying equivalent alkane carbon numbers (EACNs) and hydrophilic-lipophilic deviation (HLD) values. The detergency of oily soils with EACNs ranging from 5.2 to 16.6 was evaluated using C10-4PO-SO4Na as a primary surfactant system and a 1:1 binary mixture of C10-4PO-SO4Na and AOT as a confirmatory surfactant system (with 65/35 polyester/cotton at 25ºC). These surfactant systems were characterized using HLD concepts which showed that C10-4PO-SO4Na was more hydrophilic (had a higher negative Cc value) than that of the mixed surfactant system. Detergency of the selected soils was evaluated at different salinities corresponding to HLDs ranging from negative to positive values. The results showed that detergency of all soils increased with increasing salinity (starting with an HLD = -3 (Type I)), reached the maxima at widely different optimum salinities (Ss*) but an identical HLD value of zero (optimum Type III), and then decreased with further increasing salt levels corresponding to positive HLDs (Type II). The preferred HLD range from -3 to zero showed detergency levels exceeding 85% removal with interfacial tension values (IFTs) below 1 mNm^{-1} for all oily soils studied. Detergency of semisolid octadecane (EACN = 18) was further conducted and demonstrated that performing detergency at HLD = -3 to zero likewise revealed superior soil removal over 85% than systems outside this HLD range. Thus, this work highlighted the utility of using the HLD approach in design surfactant formulations for detergency of widely varying types of soils.

Wednesday, July 1, 2020
Session Time: 10:25 AM - 11:45 AM

Presentation Time: 10:25 AM - 10:30 AM

Track: Surfactants and Detergents

Introduction: Analytical Trace Components

Co-Chair: Scott A. Backer, Dow Chemical Co., USA - Home and Personal Care
Co-Chair: Suhkwan Soontravanich, Ecolab, USA

Trace component analysis has become an important topic in both consumer and I&I industries because of more restrictive regulations. This session focuses on analytical techniques for quantifying residual surfactants and other trace components, as well as methods and strategies to minimize residual components. The session also reviews recent and pending regulatory changes and broad industry trends that impact trace component analysis.

Wednesday, July 1, 2020
Session Time: 10:25 AM - 11:45 AM

Presentation Time: 10:55 AM - 11:20 AM

Track: Surfactants and Detergents

(4094) Approaches to achieve a manual dish detergent with low 1,4-dioxane content.

Presenting Author: Michael D. Capracotta, PhD - BASF Corp

Impending regulations will force cleaning products to contain no more than 1 ppm 1,4-dioxane by the end of 2023. This will challenge formulators to meet this criteria while maintaining performance and mitigating cost. The authors will discuss strategies in light of this new law and also present new, low 1,4-dioxane technologies that will provide a compliant manual dish detergent, without loss in performance."

Thursday, July 2, 2020
Session Time: 8:25 AM - 10:35 AM

Presentation Time: 8:55 AM - 9:20 AM

Track: Surfactants and Detergents

(4049) Certified Green Cleaning Product Performance Versus Their Conventional Counterpart

Presenting Author: Joseph Scognamiglio - SGS North America Inc.

Green cleaning products are intended to provide environmentally safer alternatives to traditional cleaning products by offering a formulation that more compatible with the environment through biodegradability and/or renewable ingredients. As such, products in this category contain a more limited scope of ingredients compared to their conventional counterparts and continue to rely on new and emerging technology to supplement their palette. In order to understand the gap in performance caused by the limited number of ingredients between green cleaning products and their conventional alternatives, products of each type were subject to standard product performance tests (Laundry Detergent, All Purpose Cleaner, Automatic Dishwasher Detergent and Hand Dish Detergent). Conventional products were selected from both National Brand and Private Label products to understand how the performance of the leading products as well as their economical equivalents would perform against sustainable and renewable products certified by the EPA Safer Choice and USDA Biopreferred programs. The results provide insight to understand the differences in product performance, which may be related to the scope of substances approved for use in their respective programs and/or the gap in technology between the conventional and green cleaning categories.

Thursday, July 2, 2020
Session Time: 10:30 AM - 12:35 PM

Presentation Time: 10:30 AM - 10:30 AM

Track: Surfactants and Detergents

(3801) Protective films of hydroxyproline rich, natural proteins improve the efficiency of hard surface cleaning formulations

Presenting Author: Eric Yezdimer, PhD - Gelita USA

Greener cleaning formulations are often not as effective as traditional harsher chemistries. However, consumers are demanding products with similar performance. Several long-term studies (e.g. for cleaning buses and trains) have shown the performance of industrial cleaners can be much improved by adding hydroxyproline rich proteins (HRPs) to their formulations. Furthermore, the environmental impact of these industrial operations could be significantly reduced, as the HRPs allowed for a reduction in the formulation's alkalinity. This work investigated the surface behavior of these proteins and their application as additives in hard-surface cleaning formulations. Quartz crystal microbalance analysis and contact angle measurements have found that dilute solutions of HRPs form net hydrophilic layers, a few nanometers thick, on different surfaces. These layers are protective and support surfactants, thus preventing soil materials from directly contacting the surface and allowing for easier sequential cleanings. The effectiveness of several cleaning formulations, with and without HRPs, were evaluated using a scrub abrasion and washability tester. Surfaces were cleaned once with their respective formulation, soiled, and then cleaned again. These experiments found that formulations with HRPs outperformed the same control formulations without HRPs. This improved performance has the potential to provide a similar or better degree of cleaning, albeit with less aggressive, more environmentally friendly chemistries. Surface tension experiments evaluating the interactions of HRPs with a series of common surfactants were also investigated. While several surfactant classes show little interaction with the HRPs, glucamine based surfactants were found to exhibit a synergistic effect with regards to their surface tensions.

Thursday, July 2, 2020
Session Time: 10:30 AM - 12:35 PM

Presentation Time: 11:20 AM - 11:45 AM

Track: Surfactants and Detergents

(4221) Predicting Microemulsions Stability, Viscosity and Cloud Points of Micelles via Spontaneous and Effective Packing Competition

Presenting Author: Thomas N. Zemb, PhD, D Sc - 3Institute for Separation Chemistry of Marcoule (ICSM) U Montpellier, CEA, CNRS

The spontaneous packing parameter is a scalar linked to accessible structures formed in solution by adjacent molecules1. The effective packing parameter of any microemulsion or micelle can be

measured by scattering2. The difference between effective and spontaneous packing creates a « frustration energy » that can moreover be evaluated in kJ/Mole by first principles3. Comparing to different types of instability in surfactant solutions allows to predict the temperature range of standardized « fish-type » phase diagrams4,5 or the differences observed upon branching of the chains in the maximum accessible temperature without micro-phase separation known as cloud-points6. The elastic energy originating from a mismatch between spontaneous and effective packing is equivalent to the more recently defined HLD when taken as an average over a whole sample7. When giant branched micelles form viscous solution, the frustration energy must be considered in terms of connexion points, end-caps and cylindrical parts of micelle-based gels that are common feature in formulated shampoos. Comparing probabilities of forming cylindrical micelles, branching points, end caps and entanglements is a general approach that can predict viscosity variations versus addition of electrolytes as well as perfumes8. Practical examples with large collection of surfactants will be shown and illustrate the parameter-free predictive power of this approach based on geometry for the curvatures and on thermodynamics with the effective "rigidity" linked to the entropy of the film, as for example in the hyperbranched surfactants 9 that are even effective in supercritical CO2.

Thursday, July 2, 2020
Session Time: 10:30 AM - 12:35 PM

Presentation Time: 11:45 AM - 11:45 AM

Track: Surfactants and Detergents

(3941) A comprehensive study of surfactant foaming stability using fluorinated and hydrocarbon surfactants

Presenting Author: Muhammad Sha Kamal - King Fahd University of Petroleum and Minerals

CO2-surfactant foam injection is a widely known enhanced oil recovery (EOR) technique that provides better hydrocarbon recovery compared to simple CO2 flooding. Selection of a suitable surfactant for foaming requires an in-depth experimental study. The surfactant should be thermally stable, compatible with reservoir brine and other chemicals, have lower adsorption on reservoir rock, have high foamability and foam stability, and should be economically viable. In this work, foamability and foam stability of three different surfactants were evaluated using a dynamic foam analyzer. These surfactants were fluorinated nonionic, fluorinated zwitterionic, and hydrocarbon zwitterionic surfactants. Effects of surfactant type and structure, concentration, temperature, polymer additions, salt addition, and type of injected gas were investigated on foamability and foam stability. The foamability was assessed using the volume of foam produced by injecting a constant volume of gas. Foam stability was determined by its half-life time. It was found that foamability was highest by a hydrocarbon zwitterionic surfactant. However, the foam generated using fluorinated zwitterionic surfactant was more stable. A mixture of solution containing zwitterionic fluorinated and hydrocarbon fluorinated surfactant showed better foam generation and foam stability. The foam that was generated using CO2 had less stability compared to air-generated foam. The addition of a polymer significantly improved foam stability

without affecting foamability. The presence of salt increases both foam stability and foam generation. This study helps in optimizing the conditions of foam injections for enhanced oil recovery.

Thursday, July 2, 2020
Session Time: 10:30 AM - 12:35 PM

Presentation Time: 12:10 PM - 12:35 PM

Track: Surfactants and Detergents

(4125) Surfactant-Polymer Association in Aqueous Media Modulated by Hydrophobicity of Surfactant, Polymer, or Solvent

Presenting Author: Paschalis Alexandridis, PhD - University at Buffalo, The State University of New York (SUNY)

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).

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

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Track: Surfactants and Detergents

(3584) Interfacial Behavior of Naphthenic Acid in Alkaline Bitumen Systems

Presenting Author: Rafael Perez-Franco - University of Toronto

The most significant barrier to achieve water-oil separation in industrial operations is the formation of highly stable water-in-oil (W/O) or oil-in-water (O/W) emulsions, known as rag layers. The stability of these emulsions is specially enhanced by the presence of naphthenic acids (NAs). NAs are a naturally-occurring mixture of carboxylic acids present in crude oil, and they can represent up to 4 wt% in bitumen. NAs can stabilize emulsions due to their amphiphilicity,

which is a function of the pH of the environment. The oil-like and surfactant-like nature of NAs, along with their dissociation to sodium naphthenates in the presence of sodium hydroxide was evaluated using the new bifunctional model introduced into the Hydrophilic-Lipophilic Deviation (HLD) framework. Using the values of HLD (at various NA neutralization levels) incorporated into the net-average curvature (NAC) framework, the interfacial tension of the diluted bitumen-water system was predicted. For the first time, the deep changes in interfacial tension observed in alkaline environment with acidic bitumen (and by extension acidic crude oils) can be fully predicted. To further explore the role of NAs, these studies were repeated at various total NA concentration in bitumen to assess the potential critical microemulsion concentration of NAs in bitumen. The relevance of the findings towards crude oil extraction and improvements in the bitumen froth processing will be discussed.

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Track: Surfactants and Detergents

(3623) A New Perspective on the Wetting of a Solid Surface by the Drops of an Emulsion

Presenting Author: Arun Ramchandran - University of Toronto

Traditionally, the wetting of a solid surface by the drop of an emulsion has been thought to be mediated by the formation of a liquid bridge that connects the drop and the surface. In the current work, we experimentally show the spreading of a drop on a surface follows a different, new mechanism. Experiments were conducted for liquid-liquid systems, wherein drops of higher density (glycerol) were allowed to settle under gravity in a lighter polymeric liquid phase (silicone oil) under conditions of small Bond numbers. The approach of the drop towards the substrate was visualized using Reflection Interference Contrast Microscopy (RICM), and the details of the film drainage dynamics and the spreading process of the drop on the surface were recorded. The temporal variation of the minimum film heights matched theoretical expectations, until the height reached few tens of nanometers, at which point a stable film was formed. Following this, deformable islands were observed to grow on the substrate, one of which eventually merged with the parent drop to complete spreading. The reasons for the arrest of film drainage and the appearance of the islands will be discussed, and also show the effect of surfactants and surface type on the wetting mechanism. The fundamental mechanism discovered here will ultimately guide the tailoring of emulsion-based coatings or paints to have predefined spreading times.

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Track: Surfactants and Detergents

(3765) Novel Dispersants for Inorganic Particles

Presenting Author: Charles O. Kerobo - BASF Corporation

The improved dispersion of inorganic particles in slurries or polymeric matrixes is one of the major challenges in many industrial and consumer applications. Examples include ceramics, pulp & paper, construction, coatings, rubber-based products and typical household applications. Finding suitable dispersants for optimum performance in a given situation could be quite complex as it depends on numerous factors such as hydrophobicity and hydrophilicity of the medium and the particles, the size and charge distribution of particles, and their concentrations amongst other variables. BASF has developed a wide range of processing aids in the form of water-soluble polymers which can enable one to design effective and efficient formulations. In this presentation, we will provide an overview of the molecular forms, mechanisms and the performance of dispersants with examples from different applications.

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Track: Surfactants and Detergents

(4099) Benign Functionalized Nanomaterials for Biomedical and Personal Care Applications

Presenting Author: Ponisseril Somasundaran - Department of Earth and Environmental Engineering, Columbia University, NY

A variety of functionalized engineered nanomaterials used for a range of biomedical applications is exposed to humans and the environment. Colloidal forces, as well as dynamic bio-physicochemical interactions, are common as the nanoparticles come across proteins, membranes, cells, DNA and organelles in humans and aquatic organisms. The colloidal forces and biochemical interactions are largely governed by the nanomaterial properties such as size, shape, surface chemistry, roughness and surface coatings/functionalization. These properties determine the dispersion stability of these nanomaterials and govern their efficacy, and post-t treatment fate. Assessment of dispersion stability necessitates the use of multiple techniques, including lifetime fluorescence, IR/Raman and Electron Spin Resonance and Nuclear magnetic resonance spectroscopy. This talk will focus on how these techniques direct the synthesis of functionalized engineered nanomaterials suitably for biomedical and personal care applications in an environmentally benign manner. As an example, this talk will discuss the assessment of the physical characteristics of diphtheria toxin mutant (CRM-197) adsorbed onto alumina phosphate

particle surfaces using a combination technique including UV-Vis, Zeta-potential, and fluorescence spectroscopy.

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Track: Surfactants and Detergents

(3729) Benefits of NRE Catalyst for Reducing 1,4 Dioxane Formation in Alcohol Ether Sulfates

Presenting Author: Tamra Weemes - Sasol Chemicals

The states of New York and California have proposed new lower regulatory limits for 1,4-dioxane that can be present in a wide range of consumer products. The New York bill S4389 proposes a limit of 2 ppm 1,4-dioxane by 2022 and 1 ppm 1,4-dioxane by 2023. These new lower limits will have a significant effect on the raw material ingredients allowed to be used in the formulated products. Formulators will need to understand the contributions each ingredient makes to the total 1,4-dioxane content of the formulation. 1,4-Dioxane is not a significant by-product of base-catalyzed alcohol ethoxylates (AE). However, 1,4-dioxane can be a significant byproduct of the acidic sulfation process to make alcohol ether sulfates (AES). There are several processing and equipment factors that can be used to control the levels of 1,4-dioxane in AES with different degrees of effectiveness and efficiencies. An additional factor that can control the level of 1,4-dioxane created during the sulfation reaction is the catalyst used to produce the ethoxylate for feed to sulfation. Our work demonstrates the effectiveness of using a Narrow Range Ethoxylation (NRE) catalyst during the production of the AE for reducing the amount of 1,4-dioxane formed during the production of the AES. As the SO3 feed mole ratio increases, the NRE-based AE produces much less 1,4-dioxane in the resulting AES. When comparing AES on the same mole ratio basis, NRE always produces less 1,4-dioxane compared to KOH-based catalyst. Higher SO3/feed mole ratios produce even more dramatic reductions of 1,4-dioxane.

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(3978) Solubilization Mechanism of Perfume Molecules in Micelles Using SAXS and NMR technologies

Presenting Author: Taku Ogura - NIKKOL GROUP Cosmos Technical Center

Solubilization of perfume molecules in micelles has been applied to the productions of toiletries, cosmetics, and beverages to aromatize these products with a transparent appearance. The structures of perfume molecules influence the solubilization state of perfumes, however, details have not been clarified yet. Understating the solubilization behavior in the micellar solution helps to give the products with novel functions. On the other hand, small-angle X-ray scattering (SAXS) enables to investigate the size and structure of micelles in solutions. In this study, we studied the solubilization state of D-limonene (LN) or Linalool (LL) in micelles formed by decaoxyethylene lauryl ether (C12EO10) aqueous solutions using the SAXS and 2D-NMR measurements. The obtained scattering data were converted to the pair distance distribution functions (PDDF) with the indirect Fourier transformation (IFT) method. The shape of PDDF curves indicates that the C12EO10 micelles swell with solubilization of LN while maintaining the spherical shape. On the other hand, shape of PDDF curves indicates that the C12EO10 micelles swell with solubilization of LL while gradually changing to the bicelle shape. Next, the PDDF curves were deconvoluted to the electron density contrast profiles. This result suggests that the LN molecules are solubilized in the micellar core and the LL molecules are solubilized in the micellar paricedo. Furthermore, the location of LN and LL in the C12EO10 micelles is evaluated by using 2D-NMR（NOESY）technique.

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(3657) Stabilizing Methyl Ester Sulfonate at Low Temperatures

Presenting Author: Atsunori Morigaki, PhD - Lion Corp

Methyl Ester Sulfonate (MES), derived from sustainable palm oil, has already been put to practical use in powder laundry detergent due to special features such as excellent biodegradability and superior detergency even at low surfactant concentrations. However, it remains difficult to apply MES to liquid detergent because of its low solubility at low temperatures. In this study, we investigated new methods of stabilizing MES in liquid detergent at low temperatures as well as the mechanism in terms of micelle structure. In our experiments,

we used C16MES. We held test solutions at -40oC and visually checked their Krafft points. We then evaluated the distribution of additives in the MES micelles from the self-diffusion coefficient, and determined the position of the additives in the micelles by monitoring where they were correlated in the MES. Finally, we evaluated micellar size by analyzing SAXS intensities using generalized indirect Fourier transformation. The Krafft point of 1% MES solution was about 35oC, which we decreased by adding a 1:1 solution of alkanol amine and aromatic sulfonic acid to MES at a ratio of 2:1. Neither was useful on its own but the synergetic effects of the different additives efficiently reduced the Krafft point. In particular, monoethanol amine (MEA) and Cumene sulfonic acid (CS) drastically decreased it to about 20oC. DOSY, NOESY and SAXS suggest that the combination of hydrophilic MEA and CS serves as a hydrophobic complex instead and promotes the distribution of MEA/CS to the micelles, enlarging micelle curvature. This may prevent MES from arranging into a crystalline structure.

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(3699) Solubility of Polyglycol Surfactants in Salt Solutions

Presenting Author: Wanglin Yu - Dow Chemical Company

Managing and enhancing solubility of surfactants in aqueous solutions that contain high concentrations of electrolytes remain a challenge in many applications, including, for example, in institutional and industrial (I&I) cleaning and agrochemical formulations. A study on water solubility of a group of polyglycol nonionic surfactants that are varied in both hydrophobe and hydrophile structures in the presence of electrolytes using a cloud point method will be described. Using high throughput methods, a large amount of cloud point data was collected on the surfactants with different structures in various electrolytes, which enabled an empirical model to be developed to predict cloud point change of polyglycol nonionic surfactants in electrolyte solutions. Predicted results by this model were in good agreement with experimental data and enable prediction of the electrolyte tolerance of these nonionic surfactants. The second part of the presentation will focus on the use of hydrotropes to enhance the solubility of polyglycol nonionic surfactants in highly concentrated salt solutions. The effectiveness of the solubility enhancement was highly dependent on chemical structure of hydrotrope. The effectiveness of a hydrotrope to increase the solubility of a surfactant also depended on the EO chain length in the surfactant. The hydrotrope-enhanced surfactant solutions at high concentrations of salt were further investigated by self-diffusion NMR technology to understand the interaction between surfactant and hydrotrope molecules in the solutions. The results suggest that, different from what was observed in a mixed anionic-nonionic surfactant solution, the hydrotropes in this study did not change the packing status of hydrocarbon chains of the nonionic surfactant in aggregates in the solutions.

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(3563) Single Unit Dose Laundry Detergents: Development and Evaluation of New Formulations

Presenting Author: Daniel T. Piorkowski, MS - Henkel Corp

Strategy and techniques for development of new Single Unit Dose Laundry Detergent to ensure proper stability and performance of new materials (solvents, surfactants, polymers). Identification and elaboration of common failure points. Methods of evaluation include film to liquid compatibility testing, water activity, pac stability testing and pac dissolution; among others. Results will be combined to show a conceptual formula that is optimized for a specific application that enables the highest possible stability at certain cost/processing constraints, while maximizing performance. Presentation will conceptually show the thought process and techniques for new formulation development for Single Unit Dose Laundry detergents and how certain chemistries may not be compatible with current systems and may require additional optimization.

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(3643) Predicting the Effect of Additives on Wormlike Micelle/Liquid Crystal Formation with Phase Inversion Phenomena

Presenting Author: Francis Choi - University of Toronto

One challenge that formulators face in the personal care industry is obtaining solutions with sufficient viscosity, for shampoos, gels, and other cosmetic products. This can be achieved in surfactant-water systems by producing nanostructures such as wormlike micelles (WLMs), branched wormlike micelles (b-WLMs) or liquid crystal dispersions (LCs) in the solution, typically by adding salt. However, the addition of fragrances or oils can disrupt the formation of these structures and the rheological response. Therefore, there is an interest in predicting the effect of such additives on the surfactant solution. The formation of these nanostructures is dependent on the interface curvature of the surfactant-oil-water system. The curvature can be identified for surfactant-oil-water systems that undergo phase inversion, with the phase inversion point corresponding to zero-curvature. In this presentation, we will show the phase inversion conditions are similar to those required for the formation of b-WLMs/LCs in surfactant-oil-water systems. Since phase inversion phenomena can be predicted with the hydrophilic-lipophilic-difference (HLD) and the net-average-curvature (NAC) frameworks, we will show the HLD-

NAC can also predict b-WLM/LC formation. To evaluate this, we obtained the phase behavior and rheology of two surfactants that produce phase inversion behavior: an alcohol propoxysulfate surfactant and sodium dihexylsulfosuccinate, in combination with a series of oils. At high oil loadings, the salinity required to produce b-WLMs/LCs matches well with the o/w to bicontinuous microemulsion transition for the corresponding systems. After, we utilize these findings to predict the impact of oils on the salt curve of a common anionic surfactant, SLES.

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(3659) Preventing Odor when Drying Clothes Indoors

Presenting Author: Masanori Fushitani - Lion Corporation

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(3728) Enhanced cleaning performance using Winsor IV microemulsions

Presenting Author: George A. Smith, PhD - Sasol

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Track: Surfactants and Detergents

(3793) Use of Radiotracer Detergency for Mechanistic Understanding of Oily Soil Removal by Nonionic Surfactants

Presenting Author: Kirk H. Raney, PhD - A&I Ventures, LLC

Radiotracer detergency has proven to be a powerful and quantitative method for investigation of detergency mechanisms. In this presentation, a consolidated review is provided of past work with this technique utilizing a variety of oily soils and surfactant blends. Radiotracer detergency from synthetic fabrics was measured using a temperature-controlled Terg-o-tometer and oily soils lightly tagged with 14C and/or tritium. Single-component nonionic surfactants and pure oils were utilized in most cases. Phase inversion temperatures of the same oil-water-surfactant

systems were measured by observing emulsion stability and microemulsion phase behavior at varying temperatures. Optimum detergency for nonpolar hydrocarbon soils was found to occur above the cloud point temperature at the phase inversion temperature (PIT) corresponding to the surfactant film composition equivalent to the added detergent composition. This finding includes both all-nonionic and nonionic-anionic surfactant blends. For nonpolar-polar soil blends such as hexadecane and oleic acid, much lower optimum temperatures were observed as the polar soil was found to act with the surfactant to form a mixed surface-active film with a low effective HLB. The radiotracer results also showed that the polar component of the soil is removed to a higher extent than the nonpolar portion. Understanding detergency mechanisms is important for the development of new cleaning systems. In conjunction with phase behavior studies, radiotracer detergency tests have provided a clear relationship between oily soil detergency with nonionic surfactant systems and the relevant PIT. Researchers should consider this technique for future basic studies of detergency and elucidation of relevant detergency mechanisms.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3821) The Molecular Origins of the Characteristic Curvature (cc) Parameter

Presenting Author: Americo Boza-Troncoso - University of Toronto

The characteristic curvature (Cc) is a term that was used to rename the 'sigma' surfactant parameter in the original HLD equation. This change was motivated by the discovery that the value of HLD represented the net curvature of the interface normalized by the inverse of a length factor proportional to the surfactant tail length. The Cc was said to be the normalized curvature that a surfactant would acquire under a set of characteristic conditions. For nonionic surfactants those conditions are: T=25C, no salt, no co-solvent, no co-surfactant added, and in the presence of an oil with an equivalent alkane carbon number (EACN) of zero, like benzene. This presentation revisits this Cc interpretation with curvature terms predicted by the Integrated Free Energy Model (IFEM) that uses the integration of free energy terms associated with oil solubilization to predict the oil solubilization radius. When the IFEM-predicted Cc values were compared with Cc values from a group contribution correlation developed from experimental data for alkyl ethoxylate surfactants, CnEj with j=3 to 6, it was observed that Cc predicted from IFEM (using the curvature definition) were consistent in trend for j<8, but IFEM predicted a nearly constant Cc for j>8. Experimental Cc values for highly ethoxylated surfactants suggest that IFEM predictions are reasonable. According to IFEM, the plateauing of the Cc value is partly due to the coil conformation of the large molecular weight polyethylene glycol group

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Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3962) Elucidation of Softening Mechanism in Rince-Cycle Fabric Softeners. -Interaction with special water in cotton fabric and softener.

Presenting Author: Takako Igarashi - Kao.Corp.

We proposed a new softening mechanism about the important role of inhibition of constructing cross-linkage type of hydrogen bonding made of bound water between cotton single fibers with the use of fabric softener. We have already introduced our original model caused by capillary adhesion force between single fiber where water on the outermost surface has an important role of cross-linker of Hydrogen bonding. This time, we tried to do direct observation of bound water on outermost surface of cotton single fiber with AFM and AFM-IR methods.With this methods,we found that interaction between bound water on cotton and softening agent have an important role of control of hardness and softness in cotton fabric.

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Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(4117) Evaluation of Extended Surfactants as Emulsifiers for Semi-synthetic Metalworking Fluid Formulations

Presenting Author: Victoria Parker - Sasol

Metalworking fluids are highly complex mixtures relying on an intricate balance of emulsifiers, oil, water, and other additives. This ratio of components is developed based on specific application requirements. Semi-synthetic type formulations are the most popular fluid for high speed applications which require rapid heat removal and efficient machining. These formulations require a stable concentrate which will form stable microemulsions when diluted to 5% to 10% in water. The concentrate and emulsion stability is directly contributed to the effectiveness of the surfactants as emulsifiers. In this study, extended surfactants are evaluated as emulsifiers for semi-synthetic metalworking fluid formulations. The effectiveness of the extended surfactants as emulsifiers is evaluated based on the foaming and the stability of the concentrate as well as the microemulsion in water of various hardness up to 540 ppm at 5, 25 and 40 oC. Concentrates were additionally evaluated based on the pH, color, viscosity, and density. The emulsion is also corrosion tested on ferrous and non-ferrous metals to ensure compatibility in the application. Surfactant parameters to be studied include the surfactant concentration, hydrophobe chain length and the number of propoxy/ethoxy groups. The results indicate that extended surfactants are excellent emulsifiers for semi-synthetic metalworking fluid formulations.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(4216) Effect of Equilibration Time on the Structural Changes of Bicontinuous Microemulsions Near Winsor-III Liquid-Liquid Interfaces

Presenting Author: Douglas G. Hayes, PhD - University of Tennessee

Bicontinuous microemulsions (BMEs), self-assembly systems consisting of oil and water nanodomains separated by surfactant monolayers, have many current and potential applications, such as for drug delivery, enhanced oil recovery, separations and purifications and media for the templating of nanomaterials and hosting of multiphasic reactions. In previous work, we discovered through use of small-angle neutron scattering (SANS) that the middle, BME, phase of Winsor-III three-phase microemulsion changes structure in the vertical direction, particularly near the lower, water-BME, liquid-liquid interface. The difference in structure will have significant implications on the performance of BMEs in separations, reactions, and for templating. We observed previously that the extent of the change differed with the equilibration time for the Winsor-III system. We recently completed SANS experiments to better understand the relationship between the structural changes in the vertical direction versus equilibration time (from 30 min to 3 weeks) and are currently processing the data. We will report on our findings in this presentation.

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Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3583) Recent Developments in the Net-Average Curvature (NAC) Model

Presenting Author: Edgar J. Acosta - University of Toronto

Over the last ten years, the NAC model (initially introduced in 2003) has seen increasing applications in reservoir modeling, formulation of drug delivery systems, formulation of viscoelastic materials, and in the design of reactive systems to produce nanoscale polymers and nanoparticles. This presentation starts with a brief review of the origin of the NAC as a scaling curvature interpretation of the hydrophilic-lipophilic-difference (HLD) empirical equations. Then, the breakthrough physical interpretation of the net and average curvature terms, and from there its application in the prediction of solubilization capacities, interfacial tension, solubilization features of ternary phase diagrams, to the prediction of wettability in submerged systems, and more recently its use in oil-free, surfactant-water systems to predict the cloud point curves and the formation of wormlike micelles and liquid crystals. As an example application in

detergency, the combination of the NAC model and flow hydrodynamics will be discussed as a tool to predict the performance of cleaning formulations.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3666) HLD Approach to Design of Surfactant Systems for Detergency of Vegetable Oils and Fats

Presenting Author: David A. Sabatini - University of Oklahoma

This presentation will look at unique challenges posed by detergency of vegetable oils and fats and the value of the HLD approach to designing surfactant systems for this application. Four vegetable oils with varying melting points (from -10 to 28 degrees C) were studied (canola, jojoba, coconut and palm kernel oils). A surfactant system of a linear C10–18PO–2EO–NaSO4 extended surfactant and a hydrophobic twin-tailed sodium dioctyl sulfosuccinate surfactant was shown to have both a desirable HLD value (near zero) and greater than 90 % detergency above the melting point of the soil. As the surfactant system varied from this optimal range the detergency performance declined. While detergency performance decreased at temperatures below the soil melting point, it was still superior to that of a commercial detergent (up to 80 vs. 40 %). More recent research has demonstrated the ability of the HLD approach to design surfactant systems for a range of soils – showing that while optimal salinities vary dramatically for widely varying soils the HLD values collapse to a common range. Thus, this presentation will demonstrate the value of the HLD approach in designing detergency systems for vegetable oils and fats.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3826) Predict Fragrance Oil Droplet Size in Personal Care Liquid Product Using the HLD-NAC Principle

Presenting Author: Hongwei Shen, PHD - Colgate-Palmolive Company

Fragrance compounds play an important role in consumer products, both for aesthetic reasons and for their antimicrobial properties. Yet, incorporation of fragrance compounds into liquid products sometimes could trigger sudden change of appearance of the product, such as inducing undesirable haziness. In this work, solubilization behavior of fragrance in surfactant liquid

system is successfully predicted based on the hydrophilic-lipophilic deviation (HLD) principle and net-average curvature (NAC) model. First of all, the equivalent alkane carbon number (EACN) of 4 targeted fragrances, and the corresponding k, Cc parameters of a ternary surfactant system were determined experimentally from microemulsion phase behavior using a reference extended surfactant, alkoxy sulfate. The HLD parameters of the ternary surfactant mixture, consisting of an anionic, a zwitterionic, and a nonionic surfactant, were also calculated separately based on the ideal mixing rule; the result is consistent with that determined experimentally. For further verification, a series of Winsor Type I (Oil-in-Water) microemulsions of fragrance oil species in surfactant systems were then created. The resulting oil droplet size was calculated based on the NAC model. The calculated size values matched well with the droplet size measured from dynamic light scattering. Impact of co-solvent ingredients dipropylene glycol and isopropyl myristate on fragrance behavior was also investigated. The HLD-NAC model shows robustness in predicting fragrance oil solubilization in complex surfactant systems. The HLD-NAC model has the potential to reduce tedious lab tests, save materials, and improve product development efficiency.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3950) Using Hydrophilic-Lipophilic Deviation (HLD) Concept in Enhanced Oil Recovery, Agrochemical and Metalworking Fluid Formulation.

Presenting Author: Thu Nguyen, BE - University of Manitoba

Having the suitable surfactant in any oil-water system is a critical parameter in most applications using oil-water systems, such as enhanced oil recovery, detergent, metalworking fluid, and agrochemical formulations. The suitable surfactants ensure proper interactions between oil and water to achieve desirable performance of such formulations. The hydrophilic-lipophilic deviation (HLD) concept was developed and modified in such a way that it had been demonstrated to be a useful tool in screening surfactants for specific formulation parameters including the salinity, temperature and oil characteristics. The HLD concept can also be used to determine the characteristic curvature, which represents the hydrophilicity/hydrophobicity, of a surfactant. It can also be used to determine the oil equivalent alkane carbon number (EACN), which represents the characteristic of the oil. Knowing these two parameters will provide a quick screening process for suitable surfactants in a desired formulation. This study demonstrates the effectiveness of using the HLD concept to screen surfactants for enhanced oil recovery formulations, validated by coreflood tests. This study also attempts to use the HLD concept to determine the EACN for base oils used in metalworking and agrochemical formulations, which will be helpful for screening effective emulsifiers for these formulations.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(4058) Effect of alkylethoxylate polydispersity on the dependence of the characteristic curvature (Cc) with surfactant concentration

Presenting Author: Sanja Natali, PhD - ExxonMobil Chemical

The Characteristic curvature (Cc) for commercial alkylethoxylate surfactants have been found to depend on the degree of polydispersity in the number of polyethylene oxide groups in the chain. This work introduces a recent bifunctional model for polar oils to explain the experimental trends. Overall, at low surfactant concentrations, a greater fraction of the ethoxymers with lower number of ethylene oxides (Low EON) tends to partition into the bulk oil phase, leaving the high EON surfactants at the interface and producing, effectively, a shift towards more negative Cc values. These effects are reported with branched alkylethoxylates and its impact on the formulation of various products is discussed.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3776) How to Improve the Sustainability of ADW Products using New Raw Materials

Presenting Author: Yvon G. Durant, PhD, MBA - Itaconix Corporation

In the past, exchanging synthetic materials for bio-based alternatives could lead to a cost increase and a loss of performance. However, there is a growing consumer demand for products with greater sustainability and this is reflected in the marketing of some leading brands. There are novel high bio content surfactants and scale inhibitors now available to formulators and this presentation will demonstrate how to incorporate them into cost effective products.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3836) Novel Laundry Additives Delivering Anti Malodor and Cooling Benefits

Presenting Author: Sanjeev K. Dey - Milliken and Company

Laundry is a complex chore that is driven by consumer's emotions. The experience of consumer laundry is driven by cleanliness, freshness and care of the clothes. With the rise in the use of polyester and polycotton fabric, consumers are dealing with malodor and wick ability issues arising from the intrinsic hydrophobic nature of the polyester fibers. The conventional way of addressing malodor is use of fragrance which works for a short period of time due to its volatility. A more robust approach to address the malodor issue would be to capture the odor causing molecules as soon as they are produced in the body rather than masking it with fragrance. The wick ability in polyester is typically introduced through a hydrophilic fiber finish on the intrinsically hydrophobic polyester fibers. During laundry the fiber finish slowly erodes, leading to a reduced performance. Leveraging Milliken's core capabilities, we have developed technologies that can provide, anti-malodor benefits and rejuvenate wicking of the fabric. These additives deposits on the fabric through the wash or via rinse cycle and provide the relevant performance. We have developed internal test protocols to validate the performance of these additives on the fabric. The talk will cover the development and validation of these additives to deliver the benefits.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3635) Separation of Water From Diluted Bitumen Emulsions with Surfactants and Fiber Coalescers

Presenting Author: Opeyemi Ajogbeje - University of Toronto

During the naphthenic froth treatment (NFT) of bitumen froth, approximately 2 wt% water is produced in diluted bitumen. This residual water contains chloride ions, which can deactivate catalysts and cause equipment corrosion. Upon centrifugation, the 2% residual water (<10 µm drops) still cannot be removed. In this work, a glass fiber coalescer was used to induce drop entrapment, coalescence, and eventual detachment of the larger drops, easily removed by gravity settling. While the method is successful, the performance depends on the operational conditions and configuration of the coalescer. The Rajagopalan-Tien (RT) version of colloid filtration theory (the most-referred version) was found to only capture some of the phenomena, but not the effect of flow velocity. This theory was modified to include coalescence probability that

accounts for the effect of interfacial tension (i.e., the effect of surfactants) and activation energy of coalescence (another parameter affected by the presence of surfactants). The new theory fully captures the effects of flow velocity, and for the first time – to our understanding – explains the empirical observations on the effects of surfactants on fiber coalescer performance. Currently, the presence of surfactants is detrimental to coalescer performance. We will discuss the use of the new theory to design surfactant-based demulsifiers that could work synergistically with fiber coalescers.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(3995) A Chemist's Guide to Formulations for the Cleaning and Care of Human Hair

Presenting Author: Perry Romanowski - Element 44 Inc

Treatments for hair represent a significant portion of the beauty industry market and are an opportunity for chemists to innovate. To that end, there are a wide variety of challenges when solving the primary problems of cleaning hair and getting it to stay in a condition that is satisfying to consumers. This talk will review the technologies and strategies formulators use to address hair cleansing, conditioning, and styling. We will explore the chemistry of surfactants, various conditioning materials, and the polymers meant to temporarily hold hair in place. We will also look at how the technology has evolved over time and where it may be headed in the future.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(4008) Skin Oils for Skin and Hair Health

Presenting Author: Apostolos Pappas, PhD - Rutgers University

The skin is the largest organ of the human body. Skin oil synthesis is one of the main skin functions and fundamental for skin health. The majority surface lipids are of sebaceous and keratinocyte origin. Their chemistry and biology seem unusual, as many skin lipids are not found in other tissues within the human body; such as unusually desaturated fatty acids, waxes and squalene (in high levels). Mainly triglycerides but also waxes and squalene are secreted by the sebaceous glands and are deposited via the hair canal on the surface of the skin. Sebaceous oil is involved in the pathogenesis of acne, seborrheic dermatitis, oily hair as well as hair loss. In

addition, more evidence has been advocating that essential dietary fatty acids and their metabolites are influencing the hair follicle and fur health. On the other hand, epidermal lipids as ceramides are fundamental for the skin barrier's properties. Recent studies have demonstrated the involvement of the epidermal oil barrier in eczema and dry skin conditions. A general practice for cosmetic chemists is to create formulations that they will proximate skin's natural barrier components, integrity and physiology. Hence, understanding the physical and biochemical elements of skin's barrier are pivotal for designing the best functional skincare products. Ceramide biomimicry, penetration limitations and their biological diversity need to be accounted towards creating the best efficacious formulations. Understanding the roles of skin lipids is fundamental for successful skincare products as well as healthy skin and hair

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(4031) How to Achieve Greater Sustainability in Hair Care with Enhanced Performance: Rescued by Ester Quats

Presenting Author: Brian Yang, PhD - Evonik Corporation

Ester quats are commonly used as softening agents in textile/fabric care industry. In contrast, their use in personal care as conditioning agents is rare and not as popular. One reason is that commonly used alkyl quats have better formulation stability and cost/performance properties. However, the growing sustainability trend is tilting the landscape towards greater use of ester quats for their biodegradability and ecotoxicity profiles, which overall are better than alkyl quats. One challenge for the ester quats is their vulnerability to hydrolysis at formulation pH common in hair care. Another challenge is achievement of a high active content while keeping the product in a favorable liquid form from a processing point of view. Thus, it is desirable to identify a suitable ester quat product that is a high active liquid, is more resistant to hydrolysis, and is able to provide comparable performance. By carefully choosing the hydrocarbon chain moiety, we were able to produce a product in liquid form with 100 percent active content. The conditioning performance was evaluated via hair tress sensory and combing equipment. It showed comparable, if not better, conditioning properties than the benchmark, Behentrimonium Chloride. Formulation wise, surprisingly, the material is not only suitable for cream rinse conditioner as one would expect, but also shows some benefits in conditioning shampoo. In the end, the test results showed that a carefully tailor-made ester quat can be a viable product for hair care and, more generally, personal care applications.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents

(4212) Cleaning Product Ingredient Disclosure: California, New York and Beyond

Presenting Author: Jacob Cassady - American Cleaning Institute

Cleaning product manufacturers are providing consumer with an extraordinary amount of ingredient information through their website. California's "Cleaning Product Right to Know Act", Senate Bill 258, requires the labeling of certain ingredients by January 1, 2021. New York Department of Environmental Conservation announced the initiation of a rulemaking process to determine what information must be reported by cleaning product manufactures and released their "recommended best management practices for cleaning product ingredient disclosure". Additional jurisdictions are likely to follow California and New York's lead and place additional disclosure requirements on cleaning product manufacturers. ACI and its member companies believe consumers should have access to information necessary to make informed choices about product purchases and that consumers have the right to understand what is in the cleaning products they use every day. Companies are meeting challenges from consumers, regulators and non-governmental organizations (NGOs) and ultimately, marketplace alignment or certainty on ingredient communication approaches will give consumers confidence that the product they purchase is safe and effective. All aspects of the cleaning product supply chain are impacted by the evolution of ingredient communication and ingredient suppliers face a unique challenge to meet the demands of their customers, cleaning product formulators. ACI provides guidance and thought leadership to member companies on how to comply with existing requirements and is involved with substantive federal and (several) state advocacy engagements on ingredient communication and transparency approaches.

Wednesday, July 1, 2020

Session Time: 10:25 AM - 11:45 AM

Presentation Time: 10:30 AM - 10:55 AM

Track: Surfactants and Detergents@@@Analytical

(4070) Trace quantitative analysis of 1,4-dioxane in care chemicals to meet regulatory challenges

Presenting Author: Cynthia K. Loop, PhD - BASF Corporation

With the U.S. Environmental Protection Agency finding very high levels of 1,4-dioxane on Long Island, NY, the New York State Legislature recently enacted the legislation "prohibiting household cleansing products, cosmetic products and personal care products that contain 1,4-dioxane". There is a requirement to have 1,4-dioxane content in these products below 2 ppm of 1,4-dioxane by 12/31/2022 and below 1 ppm 1,4-dioxane beginning 12/31/2023. Additional 1,4-

dioxane regulations are likely to crop up in other states in the near future. BASF Analytics North America developed a trace quantitative analytical method using headspace GC/FID to determine 1,4-dioxane contents in a wide range of BASF surfactant products. This analytical method supports our investigations into minimizing the 1,4-dioxane content in surfactant production.

Thursday, July 2, 2020
Session Time: 8:30 AM - 10:35 AM

Presentation Time: 8:55 AM - 9:20 AM

Track: Surfactants and Detergents@@@Analytical

(4067) Non-animal testing: what we can and can't (yet) do in vitro to ensure product safety, consumer appeal and regulatory compliance.

Presenting Author: Carol Treasure, PhD - XCellR8

Progress in non-animal testing has seen significant acceleration over the past decade. Consumer pressure has led to a number of bans and restrictions on animal testing that have fuelled this explosion of activity, leading to technical advances and regulatory approvals that may have previously seemed impossible. As an industry, we are on a continual journey to evolve more human-relevant science to ensure safe products, and to translate these technologies into practical, regulatory-compliant solutions. We are still a long way from our desired destination. This talk will provide a concise overview of which non-animal safety tests have regulatory acceptance, as well as non-regulatory methods that can be used in weight-of-evidence approaches, providing valuable information for exposure-led risk assessment of consumer products. Importantly, we'll highlight where some key challenges remain. We'll discuss how collaborative approaches are needed to overcome them, ensuring robust science to create safer-than-ever products, satisfy the regulators and meet the increasing ethical expectations of today's global consumers.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Analytical

(3641) Evaluation the Effect of Crystal Form Triglyceride on Detergency Performance

Presenting Author: Parichat Phaodee, PhD - University of Oklahoma

This work studied the effect of crystalline solid forms of tristearin (triglyceride model soil) on detergency performance at 25°C (below the melting point of tristearin) using a differential scanning calorimetry (DSC) technique. The hypothesis guiding this work was that surfactant can more readily penetrate into alpha tristearin phase due to looser packing density than the beta phase, thus facilitating the soil removal from the aluminum surface of DSC pan. Single alpha

(loosely packed) and beta (densely packed) tristearin samples were made on aluminum surface of DSC pans and detergency experiments were conducted with 0.1% C14-15-8PO-SO4Na using a terg-o-tometer. The amount of soil removal was determined gravimetrically. After the detergency experiments were completed, the DSC pans with residues were taken to analyze phase transition using the DSC – this was completed within a certain time scale to mitigate phase transition concerns. Results of these studies will provide insights into detergency of alpha versus beta form triglycerides.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Analytical

(3662) Polyetheramines in Liquid Laundry Detergents

Presenting Author: Dennis Murphy - Stepan Company

In laundry detergents, there is a continual search for additives which when used at low levels will boost cleaning performance or allow the same level of cleaning with a lower overall chemical footprint. A new class of polyetheramines has been invented which delivers against these goals. Synthesis of a particular polyetheramine molecule will be detailed followed by cleaning performance at cold, warm and hot wash temperatures against a broad spectrum of stains in model formulations. A hypothesis on how the technology works will be presented along with data to support the hypothesis.

Tuesday, June 30, 2020

Session Time: 11:45 AM - 1:00 PM

Presentation Time: 11:45 AM - 12:10 PM

Track: Surfactants and Detergents@@@Biotechnology

(3975) Multi-Functional Bio-Based Polymers in Laundry Detergents Prevent Staining and Graying

Presenting Author: Rodrigo MenaBrito - Clariant Corporation

Fabrics made from polyester and polyester/cotton can be difficult to clean when they are soiled with oily or fatty stains. Such stains adhere strongly to the hydrophobic synthetic fibers, which are then only poorly wetted by the washing liquor. If these fabrics are washed with a detergent containing a soil release polymer, the soil release polyester is adsorbed onto the hydrophobic fibers and forms a hydrophilic film. This prevents the soil from adhering directly to the fibers. Furthermore, the affinity of hydrophobic soils for the hydrophilic film is reduced significantly compared to the untreated fibers. This makes it much easier to remove oily stains from the fabric during subsequent washing. With the Soil Release Polymer, we developed a solution which meet

high sustainability standards and function in several different ways: They remove stains even at low temperatures and short cycles, protect against new soiling, reduce graying and improve wearing comfort by increasing moisture absorption. The new polymer is 80% bio-based and has the same performance compared to the previous synthetic generation.

Thursday, July 2, 2020
Session Time: 8:25 AM - 10:35 AM

Presentation Time: 9:20 AM - 9:45 AM

Track: Surfactants and Detergents@@@Biotechnology

(4090) Hemp Oil Ethoxylates for Home and Personal Care Applications

Presenting Author: George A. Smith, PhD - Sasol

Hemp is a strain of cannabis sativa plant grown for industrial use. Hemp is used commercially to make rope, paper, textiles, fiber board and building insulation. Hemp oil is obtained by pressing hemp seeds. Cold pressed hemp oil is light colored with a nutty flavor. Hemp oil is rich in linolenic fatty acids and is used to make biodiesel, drying oils for paints and coatings and in nutrition and animal feed. Work has been performed to use hemp oil as a feedstock to make water soluble surfactants for home and personal care applications. By reacting the oil with a polyol, a variety of different nonionic surfactants can be prepared such as fatty acid ethoxylates, methyl ester ethoxylates and vegetable oil ethoxylates. The surface properties on hemp oil ethoxylates have been evaluated. In general, hemp oil ethoxylates show low CMC and surface tension. They show good interfacial tension reduction and detergency in textile cleaning applications. Hemp oil ethoxylates are good foam stabilizers for liquid dish, shampoo and body wash.

Thursday, July 2, 2020
Session Time: 8:25 AM - 10:35 AM

Presentation Time: 9:45 AM - 10:10 AM

Track: Surfactants and Detergents@@@Biotechnology

(3787) Microbial glycolipid biosurfactants: from self-assembly to hydrogel and emulsion development

Presenting Author: Niki Baccile - Sorbonne Université / CNRS

Soft self-assembled materials (hydrogels, coacervates…) are applied in many fields, from thickeners, to drug encapsulation, wound healing, etc… Microbial glycolipid biosurfactants, obtained from the fermentation of renewable resources and interesting for their biodegradability and low cytotoxicity, may constitute a new class of soft materials. However, their self-assembly properties are still poorly known [1,2] and their applications in the field of soft matter practically

not existing. This contribution discusses the self-assembly properties of selected microbial glycolipid biosurfactants and the recent development of soft materials. We show that microbial glycolipid biosurfactants can form self-assembled micelles, fibers and bilayers, that can then be used to form hydrogels in water [3], coacervates [4] or emulsions, the properties of which will in turn depend on pH and temperature. The self-assembly will be shown via SAXS and cryo-TEM experiments, while the gelling properties will be analyzed using time, temperature and pH-resolved rheology experiments. This presentation provides a new insight in terms of understanding the complexity of the physico-chemical behaviour of microbial glycolipid biosurfactants but it also shows that understanding their properties allows their use in the preparation of soft materials. 1 A.-S. Cuvier, N. Baccile et al. Soft Matter, 2014, 10, 3950 2 N. Baccile et al. Langmuir, 2016, 32, 6343 3 N. Baccile et al. Soft Matter, 2018, 14, 7859 4 G. Ben Messaoud et al. Green Chemistry, 2018, 20, 3371

Thursday, July 2, 2020
Session Time: 8:30 AM - 10:35 AM

Presentation Time: 10:10 AM - 10:35 AM

Track: Surfactants and Detergents@@@Biotechnology

(3555) Cationic Inulin – The Next Generation Ingredient for 2-in-1 Laundry Detergents

Presenting Author: Robert Nolles - Cosun Biobased Experts

The ingredient A new range of quaternary polymers was developed through the functionalization of inulin, which is a naturally occurring polysaccharide extracted from chicory. The high reactivity of the inulin backbone allows much higher degrees of substitution (resulting in higher charge densities) than can be achieved with cellulose and guar. Another advantage of using inulin as a backbone is that it results in an inherently biodegradable ingredient, which complies with the trends in the home and fabric care industry. **High performance at low use level** The main purpose of cationic polymers is to neutralize negative charges on fabric. Our research has shown that cationic inulin demonstrates excellent softening in combination with a significant static reduction effect in 2-1 laundry detergents, at use levels >50% lower than typical cationic polymers such as PQ-10 and cationic guar. Moreover, studies indicated that cationic inulin helps to drive silicone oil to the fabric, enhancing performance. Lastly, fundamental research showed that cationic inulin has high efficacy in depositing surfactants onto hydrophilic surfaces, most likely due to strong coacervation behavior. **Easier to use than alternatives** Since cationic inulin is very water-soluble, it is easy to formulate with: no heating nor pH adjustment is required to incorporate it in a formulation. Furthermore, its compatibility with a wide range of surfactants makes it convenient to use in 2-in-1 detergents. **Conclusion** Cationic inulin can be considered thé next generation ingredient for fabric softening, particularly suitable for use in 2-in-1 laundry detergents: high performing, user-friendly and sustainable.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Biotechnology

(3624) Production of Fatty Alcohols from Biomass-derived Chemicals Using Chemo-catalytic and Bio-catalytic Pathways

Presenting Author: Dimitris I. Collias, PhD - Procter & Gamble

Fatty alcohols can be produced via either a chemo–catalytic or a bio-catalytic pathway from biomass-derived chemicals, such as, sugars, methyl furfural, acids, ketones, and aldehydes. After a detailed description of the two pathways, we will compare them in terms of process conditions and estimated economics. In the chemo-catalytic pathway, a stepwise process was developed that first builds the carbon skeleton from biomass-derived chemicals to a targeted structure and length, which is then followed by a selective removal of all but the acid or ester group. This process is exemplified in the making of methyl-dodecanoate from a carbon skeleton containing furan, alkene, ketone, and ester functionalities. The catalyst selection for the selective removal step will be described in detail. Some catalysts were able to effectively catalyze this reaction under specific conditions (temperature and space velocity) without over-reacting the acid or ester product to alkanes. In the bio-catalytic pathway, sugars were selectively converted in a single step fermentation to C12 and C14 fatty alcohols. The conversion was catalyzed by a genetically engineered strain of E. coli, whose natural fatty acid biosynthesis pathway was highly upregulated and diverted into a novel fatty alcohol biosynthesis pathway. The novel pathway was composed of a thioesterase, fatty acid carboxylic acid reductase, and aldehyde reductase. The fermentation process approached 80% of theoretical yield, was successfully scaled in a 132,000 L demonstration scale bioreactor, and was included in a Presidential Green Chemistry award made to LS9 in 2010.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Biotechnology

(4051) Application of sophorolipid technology with glycerin gel in cosmetics

Presenting Author: Glen Lelyn Quan, MS - Saraya Co., Ltd.

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 gelling property, which can be used in cosmetics. Glycerin is commonly used in cosmetics and personal care products as humectant, and comes third after water and fragrance as the most frequently used cosmetic ingredient. However, its fluidity sometimes causes difficulty for it to be used in other formulations. This investigation focused on the gelation attempt of glycerin using

sophorolipids and its application in cosmetics. Investigation of surfactants used in cosmetics including sophorolipids was performed to confirm which can create glycerin gel. From the results, it was confirmed that gel formation of glycerin could be achieved with sophorolipids. The results were further evaluated using scanning electron microscopy, where a densely structured network of glycerin and sophorolipids was confirmed. Applying this technology in cosmetics, glycerin gel was able to create a thermally irreversible stable glycerin gel network with any oil even without other additives. This sophorolipid technology could help achieve simpler and cleaner cosmetics and personal care products in the future.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Biotechnology

(3722) Recent Advances in Enzyme Technology Leading to Greater Formulation Flexibility and Cleaning-Product Performance

Presenting Author: Thomas J. Burns - Novozymes North America, Inc.

In recent years, a new generation of enzyme products has been developed. With this, many of the conventional obstacles to formulating effective enzymatic cleaning products have been overcome. We will review the advances in biotechnology and ancillary ingredients incorporated in these improved enzyme preparations, which now allow formulation flexibility beyond the traditional restrictions and taboos associated with successful use of enzymes as ingredients. Further, this talk will dispel many of the myths surrounding effective use of enzymes, and point to novel combinations of ingredients permitting broader product efficacy than has previously been possible.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Biotechnology

(3719) Keep your friends close & your microbes closer: Changing our perception of what 'cleaning' means

Presenting Author: John R. Harp - Novozymes

Microorganisms have a long history of being the enemy when it comes to human health and disease. Consequently, we take pride in killing these microbes when we clean our homes and even our bodies. What if we changed our mindset from killing and instead, embraced microbes as a beneficial part of our lives? More and more data are published regarding the beneficial

nature of microbial life in terms of human health. We see that exposure to microbes early in life helps nurture our immune system, such that it responds appropriately to challenges. Given this connection, it is time to start thinking about how we can live in harmony with our microbial neighbors instead of thinking of them as invaders. In this study, we explore the diversity of microbes present on various surfaces in homes to understand the dominant species associated with the home environment. Moreover, we investigated how using a probiotic based cleaning solution modulated the home environment. By assessing various sampling methods, we determined that no surface in the home is free from microbial life, albeit some surfaces are more populated with microbes than others. Further, we found that the probiotic cleaning solution supported the probiotics in bottle and that once applied, allowed for the potential to balance the ecology of home surfaces. These data suggest that applying a probiotic based cleaning solution can introduce a high number of probiotic microbes that have the capacity to clean while providing an alternative to the harsh chemistries that we currently use.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Biotechnology

(3713) Probiotic Cleaning - Shifting the Paradigm

Presenting Author: Hilary J. Cheeseman - Novozymes North America, Inc.

Humans spend more than 90% of their lives indoors. In the home, we are exposed to a plethora of dirt, debris and microscopic life. We are often overly enthusiastic about making our lives as clean as possible and ultimately that involves targeting and killing the microbes around us with harsh chemicals. In scientific literature, evidence is piling up that suggests microbes promote and support human health. Why do we consider these organisms an enemy? Instead, Novozymes and the industry aims to shift the way we think about what clean means by harnessing the natural cleaning power of microbes. In this study, we tested and validated cleaning chemistry that is compatible with and allows probiotics to be a key ingredient of hard surface cleaners. Formulating cleaners around the probiotics is the key to unlocking their power. With cleaning technology that supports the diversity of microbes in our homes but allows us to tackle soils immediately upon application, we can achieve a long-lasting clean. We can change how we clean our homes by embracing microbes instead of killing them. We will share data that demonstrates how chemistry can impact spores in a formulation, how active probiotics excrete enzymes for cleaning, and how technology can respond to the presence of soils on a surface and transform from a dormant spore state to active probiotics.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Biotechnology

(3813) The Evolving of Detergent Formulations and Keys to Keeping Enzymes Active

Presenting Author: Hendrik Hellmuth - AB Enzymes GmbH

Detergents are composed of various different ingredients. To achieve the best possible performance, these materials have to be designed and formulated in a way that they work synergistically, and don't hinder each other in their actions. Enzymes are a well-established ingredient of modern detergents, but are known to be prone to inactivation. Therefore, the compatibility of Detergent Enzymes with other ingredients was always carefully monitored, and several countermeasures were taken into account in formulating enzyme containing detergents. With new types of formulations and product categories, however, new challenges and constraints have to be taken into account. Here, we review mechanisms behind enzyme inactivation, ways to counter such degradation in the formulation, and how enzyme design of AB Enzymes' newest enzymes can increase general enzyme stability, giving you worry-free high-performance and full flexibility to optimize your formulation.

Friday, January 1, 2021

Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Edible Applications Technology

(3472) Fabrication and Characterization of W/O/W Emulsions with Surfactants and Crystalline Lipid Phase

Presenting Author: Jinning Liu - University of Massachusetts, Amherst

Multiple emulsions have considerable potential for the encapsulation, protection, and controlled release of hydrophilic functional ingredients. In this study, we fabricated anthocyanin-loaded W/O/W emulsions in which the lipid phase was crystalline. Anthocyanin was used as a model hydrophilic ingredient because it is a natural food colorant and nutraceutical that is highly susceptible to degradation, which leads to color fading and loss of bioactivity. Polyglycerol polyricinoleate (PGPR) was used as a lipophilic surfactant to stabilize the inner water droplets, while quillaja saponin was used as a hydrophilic surfactant to coat the oil droplets. Gum Arabic was also incorporated into the outer aqueous phase as a biopolymer surfactant. Hydrogenated soybean oil (HSO) was used to create the crystalline lipid phase with the intention of inhibiting leakage of the anthocyanin from the inner aqueous phase. In general, the W/O/W emulsions formed were highly susceptible to droplet aggregation, which led to a large increase in viscosity. The rheology and stability of the emulsions depended on the level of gum arabic, PGPR, and

quillaja saponin they contained. Gum arabic appeared to inhibit droplet aggregation and thickening, which was attributed to its ability to form a protective coating around the W/O droplets. Conversely, PGPR appeared to promote droplet aggregation, which may have been due to its ability to adsorb to the fat crystal surfaces and change their location or interactions. Overall, our results provide some useful insights into the formulation of double emulsions together with the surfactants for the encapsulation of hydrophilic bioactive agents.

Wednesday, July 1, 2020

Session Time: 10:25 AM - 12:35 PM

Presentation Time: 11:45 AM - 12:10 PM

Track: Surfactants and Detergents@@@Health and Nutrition

(3942) Plant Lipid Classes in Skin Care

Presenting Author: Benjamin Schwartz - AAK USA

This will be a brief overview of the different classes of plant-based lipids used in skin care products as a means of replenishing the barrier function of the epidermis. Regular cleansing of the skin is necessary for hygienic purposes, however cleansing surfactants remove the oily layer of lipids secreted onto the skin by the sebaceous glands, as well as some of the structural lipids of the stratum corneum. Additionally, extreme environmental conditions or skin disorders can stress or alter the lipid composition of the epidermis. Thus, most traditional skin care products are a means of providing the outer layer of the skin with lipids similar to those produced by the body itself. Use of these skin care products helps to prevent the unwanted side effects of regular cleansing and exfoliation, as well as the effects of environmental or biological stresses, such as dryness, irritation, chapping, flaking, etc. We will discuss triacylglycerols/triglycerides (fats and oils), wax esters, terpenes, sterols/sterol esters, fatty acids, phospholipids, and ceramides. Additionally, as we go through these categories, we will briefly touch on some of the differences between the composition of native skin lipids and the corresponding plant-based versions used in skin care products.

Wednesday, July 1, 2020
Session Time: 10:25 AM - 12:35 PM

Presentation Time: 12:10 PM - 12:35 PM

Track: Surfactants and Detergents@@@Health and Nutrition

(3953) Significance of Surfactant Selection in Skincare Sensory

Presenting Author: Mark Chandler - ACT Solutions Corp

Objective/Hypothesis Formulators of skincare emulsions have 3 objectives: Stability, Sensation, and Superiority. The first is a given and takes skill to accommodate the challenges of an ever-changing consumer marketplace and fears over the safety of many (safe) ingredients. The third is usually handled by cosmetic active ingredients which ultimately assist in making the skin look more attractive. The sensory part has been seen as the easiest of the three, approached primarily by mixing and matching emollient oils for intended tactile sensations. This presentation will challenge this notion and challenge formulators to get better at the basics of making oil and water peacefully coexist, and to be bold in exploring alternative ways to make this happen. Methods Used Expert panels from Sensory Spectrum were used to evaluate roughly 30 sensory attributes of emulsions. Both emollient oil and emulsifier were varied in the study outlined by Wiechers. Discussion on emulsion stabilization mechanisms and formulation techniques are taken from a lifetime of study of the work from such notables as Tadros, Friberg, Griffin, Dederen, Klein, and others. Results Emollient selection has influence on the After-feel of skincare emulsions, but surfactant emulsifier selection has control of Appearance, Pick-up, and Rub-out, plus an equal influence to emollient on After-feel. Conclusions Formulators of skincare emulsions need to get better at understanding the range of emulsifiers and stabilization mechanisms available to them .

Thursday, July 2, 2020
Session Time: 8:30 AM - 10:35 AM

Presentation Time: 9:45 AM - 10:10 AM

Track: Surfactants and Detergents@@@Health and Nutrition

(3785) Extending Colligative Properties to Short Chain Alcohols using HLD

Presenting Author: Michael Warren - The University of Oklahoma

Short chain alcohols are used in numerous applications such as drug delivery, detergency and EOR involving ionic and nonionic surfactants. Commonly used as a “co-surfactant” or “co-solvent”, short chain alcohols like methanol to butanol can act in some ways like a surfactant, adsorbing to interfaces and lowering surface tensions. Unlike surfactants, these molecules cannot form micelles but interestingly can self-associate in water based on the hydrophobicity of the alcohol. When used in conjunction with various surfactants, changes in formulation phase behavior and notable properties such as oil solubilization have been observed. In order to further understand the effects of such alcohols on formulation behavior, we employed the Hydrophilic Lipophilic Deviation (HLD) model in order to quantify the changes in formulation HLD

parameters, K and Cc, as a function of alcohol concentration. Preliminary results for two reference surfactants have confirmed previous work done by the Salager group and imply that there exists a minimum hydrophobe size (n-propyl alkyl) in order to interact within the palisade layer. Further, by following Ostwald's logic of molar properties we propose a modification to the HLD f(A) term where the additive properties of the alcohol such as its size (molecular weight) and hydration can predict the effect on the formulation HLD. This modification conveniently returns HLD to a colligative equation in which the changes of surfactant chemical activity is only a function of solute concentration (in g/100ml) and temperature.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Health and Nutrition

(3865) Hazard/risk Assessment Approach to 'new' Chemicals Registration Under Tsca Reform

Presenting Author: Edwin C. Bisinger, Jr., PhD - Itaconix Corporation

A key part of the U.S. Toxic Substances Control Act (TSCA) is the requirement that "new" chemical substances must be evaluated by the U.S. EPA prior to commercialization in the United States. In 2016, TSCA was amended or "reformed" by the Lautenberg Chemical Safety Act and the U.S. EPA is now required to make an affirmative finding on the safety of each "new" chemical before it is allowed into the marketplace, resulting in regulatory restrictions on the marketing of many "new chemical substances. A hazard/risk assessment process can assist companies and reduce their regulatory burdens when commercializing "new" chemicals under TSCA. This comprehensive process also incorporates green chemistry when developing "new" chemical substances.

Thursday, July 2, 2020

Session Time: 8:30 AM - 10:35 AM

Presentation Time: 9:20 AM - 9:45 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(4113) Impacts of Recent U.S. TSCA Changes

Presenting Author: Thomas C. Berger, JD - Keller and Heckman LLP

The Toxic Substances Control Act (TSCA) (15 U.S.C. § 2601 et seq.), initially enacted in 1976, is the general chemical control law in the United States. TSCA regulates the manufacture, import, processing, distribution, use, and export of non-exempt "chemical substances," including detergents and surfactants. TSCA is administered by the U.S. Environmental Protection Agency

(EPA). The “Frank R. Lautenberg Chemical Safety for the 21st Century Act” (LCSA) was enacted on June 22, 2016, and significantly modified TSCA. The LCSA provided for modified as well as new authority for EPA to review and regulate new and existing chemicals in U.S. commerce. TSCA provides for the testing (section 4), premanufacture notification (section 5), regulation (sections 6, 7), and reporting (sections 8, 12, and 13) of new and existing non-exempt chemicals. Although the LCSA amended the majority of the substantive sections of TSCA, the law’s changes to section 5, 6, and 8(b) have had the most significant practical impact. EPA’s post-LCSA section 5 premanufacture notification (PMN) process is significantly different, the Agency is in the midst of prioritizing, assessing, and regulating new “high priority” chemicals under section 6, and the TSCA section 8(b) Inventory “reset” requirements impose new obligations on “inactive” chemicals. Violations of TSCA are subject to enforcement and substantial monetary penalties. In addition, TSCA non-compliance can require immediate cessation of commercial activities. TSCA compliance is further complicated by complex and often unpublished nomenclature rules. Companies conducting business in the U.S. would be well-advised to take steps to diligently comply with TSCA.

Thursday, July 2, 2020
Session Time: 10:30 AM - 12:35 PM

Presentation Time: 10:55 AM - 11:20 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3840) Construction of Pseudoternary Phase Diagram and Stability of Microemulsion from Castor Oil

Presenting Author: Chintya Gunarto - National Taiwan University of Science and Technology

Microemulsion (ME) is a one phase-transparent system, containing oil and water phases with surfactant/cosurfactant assistance to lower the surface tension. Recently, ME is widely used in biomedical application for prolonging drug delivery in human body. In this work, castor oil, tween 80 or tween 20 as the surfactant, glycerol or ethanol as the co-surfactant, and DI water as the water phase for ME preparation was studied by phase titration method. The effect of surfactant to cosurfactant ratio on the pseudo ternary phase diagram was investigated. A ratio of tween 80 to ethanol = 4/1 (w/w) resulted in the largest ME area in the pseudo ternary phase diagram. ME with tween as the surfactant and ethanol as the cosurfactant showed better stability according to their particle size and polydispersity index. It was found that 35-day storage and centrifugation did not have effect on the stability of the ME.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3838) The Development of New Surfactants and Dispersants for Automatic Dishwashing

Presenting Author: Eric P. Wasserman, PhD - Dow Chemical Company

Recent restrictions on the use of phosphate builders in automatic dishwashing detergents cause them to struggle to provide low filming and spotting on dishware at reasonable cost. Low-cloud point nonionic surfactants can improve the economics of shine by enabling formulators to use a wider range of builder combinations to maintain low spotting on dishware surfaces. Recent work at Dow has found that certain capped surfactants show particularly strong spot inhibition even in formulations free of expensive aminocarboxylate builders. A third surfactant has been developed for applications in which a liquid format is required. Possible mechanisms for their action in dishwashers will be discussed. Dow has also been active in the development of new dispersants that thrive in the low-aminocarboxylate environment, and our talk will conclude with a review of one of them, a hydrophobe-modified polyacrylate.

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Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3613) Application of a New Class of Triglyceride Ethoxylates in Agrochemical Formulations

Presenting Author: Bhaskar M. Ramachandran - Sasol

Base catalyzed castor oil ethoxylates are an industry standard product, generally used as emulsifiers in various agrochemical formulations like emulsifiable concentrates, micro-emulsions, etc. A new class of triglyceride ethoxylates useful in agrochemical formulations, which has several advantages of the industry standard, has been identified. The objective of the study was to identify the advantages of this new class of triglyceride ethoxylates over the industry standard. A systematic comparison of the industry standard castor oil ethoxylates and the new class of triglyceride ethoxylates, showed that the new class of triglyceride ethoxylates has similar emulsification and product stabilization characteristics, but has other significantly improved physical and chemical properties which are desired in agrochemical applications. The findings from the study clearly indicate the potential application of the new class of triglyceride ethoxylates as an attractive alternative to the industry standard in agrochemical applications.

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Track: Surfactants and Detergents@@@Industrial Oil Products

(3650) Nonlinear mixing rules in HLD with interacting surfactants allow to widen optimum formulation ranges

Presenting Author: Ana M. Forgiarini - Universidad de los Andes de Venezuela.

It has been known for a long time that mixtures ot similar surfactants often behave as pure substances as far as the HLD equation is concerned. However, if there are particular interactions between two or more surfactants, an extremely non-linear mixing rule could happen with quite uncertain predictions in formulation and performance. Nevertheless such nonlinearity may result in curious optimum formulation double occurrence, sometimes with close compositions. This could result in a mixture range with little variation of the HLD, thus in relatively wide optimum formulation zones which are unlikely to happen in most systems. This could be an advantage for some applications for which spontaneous formulation changes often happen

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Track: Surfactants and Detergents@@@Industrial Oil Products

(3664) Isomeric effect of linear secondary alcohol ethoxylates on surfactant performance

Presenting Author: Sung-Yu Ku, PhD - Dow Chemical Company

In alcohol ethoxylate nonionic surfactants, the properties and application of surfactant products are largely dependent on hydrophobe structures. Linear secondary alcohol ethoxylates (SAEs) have demonstrated performance advantages, such as better wetting, less stable foam, and improved handling properties, over primary alcohol ethoxylates (PAEs), and proven to be readily biodegradable. In an SAE molecule, the ether linkage connecting the polyethylene glycol chain and the alcohol can be varied along the hydrocarbon chain in the alcohol moiety, which causes various isomeric structures. The isomeric structure variations may affect the properties of the resulting SAE surfactant products. In this study, a series of SAE surfactants were produced and the isomeric structures with different ether linkage positions were characterized by NMR techniques. The product samples include those that have the ether linkage positions randomly distributed along the hydrocarbon chain and that have the linkages concentrated at the C-2 position, as well as those with the linkage distribution profiles in between. The SAE surfactant products with different ether linkage distribution profiles were compared for their physical and surface properties, including solubility and gelation behavior in water, surface tension, critical micelle concentration (CMC), dynamic surface tension, wetting properties, and foaming

properties. The materials were further compared for their performance on hard surface cleaning and emulsification to oils.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(4007) High mole ethoxylates as potential drift reduction agents

Presenting Author: Bhaskar M. Ramachandran - Sasol

High mole ethoxylates as potential drift reduction agents Bhaskar M. Ramachandran, Nomihla Valashiya-Mdleleni, Brent Lambert Sasol Performance Chemicals Agricultural spray drift is one of the biggest concerns in agrochemicals today due to resurgence of actives like 2,4-D, Dicamba, the introduction of glyphosate resistant seed traits and the growing use of drones for spray application. Commonly used drift reduction agents (DRA) include polymer based (Gaur, acrylamides) and oil/emulsion based (seed oil, mineral oil etc.) products. The objective of this ongoing study is to evaluate if high mole ethoxylates (HME) based on different hydrophobes and blends of HME and fatty alcohols provide any activity as a DRA. Preliminary test results and future drift tunnel testing plans will be presented.

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Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3646) Remembering origin and avoiding confusion in the SOW formulation expression HLD for optimum formulation

Presenting Author: Jean-Louis L. Salager, PhD - FIRP Laboratory

Winsor proposed in the 1950 a way to express the formulation effects in surfactant-oil-water (SOW) systems as the ratio of interfacial interactions of S with O and W. EOR studies in the 1970's introduced the formulation unidimensional scan method and the optimum formulation event corresponding to the occurrence of a WIII diagram and a minimum interfacial tension. Then, a surfactant affinity difference SAD equivalent to Winsor's R was shown to exhibits linearity in many double scan experiments. Around 2000, the currently used basic concept HLD (Hydrophilic Lipophilic Difference) was suggested as a generalized formulation tool. The interpretation of the surfactant contribution was proposed to be determined in different ways, sometimes misleading, which have to be cleared. A simple mathematical discussion shows how

to interpret the old and current experimental data and how to handle a normalized HLD to avoid confusions and to use the formulation concept in pratice.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3652) Improving the performance of a SOW system in petroleum applications by using multiple formulation changes

Presenting Author: Jean-Louis L. Salager, PhD - FIRP Laboratory

Surfactant-oil-water complex systems are found in enhanced oil recovery or crude oil deshydration, and other petroleum applications. A best performance is found somewhere in a typical unidimensional formulation scan, whatever the used variable in the surfactant-oil-water system, e.g. oil nature (EACN), aqueous phase salinity, surfactant head and tail, temperature and pressure. A performance comparison between two cases requires to be at the so-called optimum (HLD=0) in both situations, and thus it is necessary to change (at least) two formulation variables. Some pairs of changes are more effective than others in improving performance, and some trends have been found. Nevertheless, there are a few unexplained exceptions to the most logical occurrence proposed by Winsor in the 1950's

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Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3782) Enhanced Oil Recovery: Lessons and Opportunities

Presenting Author: Jeffrey Harwell, PhD - The University of Oklahoma

Billions of barrels of unproduced oil from known reservoirs constitute the lure of enhanced oil recovery. For nearly 50 years researchers from around the world have sought to realize the potential of this resource. The current state-of-the-art for surfactant EOR is examined in light of its failure to have a major impact on energy production and opportunities for innovation are proposed. Additionally, spinoffs from the decades of EOR research are presented in light of their impact on other areas of science and technology.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3792) Study the Effect of Linear and Branched Hydrophobic Tail and Spacer Group on the Physicochemical Properties of the Synthesized Gemini Surfactants for Enhanced Oil Recovery

Presenting Author: Syed S. Hussain - King Fahd University of Petroleum and Minerals

The estimated temperature of the carbonate rocks is around 100 oC and the salinity ranged up to 240,000 ppm. Surfactants tends to reduce interfacial tension and alter rocks wettability. However, surfactants can be precipitated while encounter with reservoir ions at elevated temperature. The thermal stability and solubility of the surfactants is the major concern. To address the issues, a series of cationic gemini surfactants with linear and branched hydrophobic tail and different spacer groups were synthesized. The chemical structure was confirmed by MALDI-TOF MS, 1H NMR, 13C NMR, and FTIR spectrometry. Short and long period thermal stabilities were measured using thermal gravimetric analysis and aging technique respectively. Interfacial and surface tension were investigated by spinning drop method and pendant drop technique respectively. Rheological data was obtained with the aid of discovery hybrid rheometer (DHR-3). The synthesized cationic gemini surfactants exhibited higher short period and long period thermal stabilities. Linear and branched hydrophobic tail showed significant impact on physicochemical properties. The synthesized surfactants showed excellent solubility in water and the critical micelle concentration, the corresponding surface tension, as well as interfacial tension values were comparable or higher to the commercial surfactants. The rheological measurements revealed that the storage modulus was reduced by enhancing surfactant concentration at lower shear and frequency because of chemical interaction and charge screening. The developed cationic gemini surfactants exhibited higher thermal stabilities and excellent surface activities including surface tension, interfacial tension, and rheological properties and revealed great potential in high salinity high temperature carbonate reservoirs.

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Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Industrial Oil Products

(3707) A New Green Solvent for Aqueous Cleaning Formulations

Presenting Author: Scott Jaynes, PhD - Croda Inc

Formulators of non-toxic, sustainable cleaning products have limited choices when choosing a water compatible solvent. Traditional glycol ethers can have measurable VOC's or toxicity concerns and do not contain significant bio-based content. D-Limonene is plant based, but also has VOC concerns and is difficult to solubilize. More recently developed green solvents meet some sustainability criteria but often provide only moderate cleaning performance or may have other drawbacks such as bad odors or aquatic toxicity. We now introduce a new class of ester-based solvent with high compatibility in aqueous cleaning formulations, excellent cleaning performance and a safe and sustainable product profile. The new family of solvents is prepared from plant-based starting materials with a final bio-based content of ~80%. The products are readily biodegradable, non-irritating, VOC exempt and exhibit low aquatic toxicity. Performance testing of the solvents at only 0.5-2% in aqueous cleaning formulations exhibited significant improvements in the removal of greasy soils versus surfactant-based cleaners alone. Benchmarking against competitive technologies showed the cleaning performance to match or exceed other available solvents on a variety of mixed or greasy soils. The new solvents were found to be effective in applications including household and institutional cleaning, industrial degreasing, and oil and gas cleaning operations. This new green solvent provides an opportunity to replace high VOC, high solvent cleaners with safe, sustainable aqueous based formulations that still deliver excellent cleaning performance.

Monday, June 29, 2020

Session Time: 8:25 AM - 10:10 AM

Presentation Time: 9:45 AM - 9:45 AM

Track: Surfactants and Detergents@@@Processing

(4042) Digitalization of formulation developments via HLD-NAC

Presenting Author: Sander van Loon, MSc - VLCI

The applied predictive formulation science, Hydrophilic Lipophilic Difference – Net Average Curvature (HLD-NAC) is very powerful to find matching ingredients, resulting in improved stability and efficacy of end-products. Although it has been applied for many years, there is still a limited use in formulation developments and ingredients thereof. The equation requires practical parameters of surfactants and oils. Once generated, compatible combinations can be predicted to develop and optimize specific formulations. The ingredient parameters generated via

the model are predictive and sustainable: you can use them over and over, allowing you to move away from trial-and-error and use digitalization in product developments. This is a very efficient way to enhance the properties in addition to reducing the complexity, time and cost of developing formulations or ingredients. When combined with High Throughput (HT) screening for automated, parallel and small-scale preparation of samples and end-products, further efficiencies can be achieved. The HLD-NAC approach and the required ingredient parameters will be explained via practical applications to showcase how it can lead to efficient developments of a broad range of products. The use of HT screening will be explained as well and why this is needed to fill up the ingredient database of our HLD-NAC app. This app can be used as the first stage of experimentation by formulating emulsions digitally, followed by a drastically streamlined amount of practical lab work needed, compared to trial-and-error. This digital HLD-NAC approach will be demonstrated, to show how this can boost efficient emulsion and ingredient developments.

Thursday, July 2, 2020
Session Time: 8:30 AM - 10:35 AM

Presentation Time: 8:30 AM - 8:55 AM

Track: Surfactants and Detergents@@@Processing

(3994) CELLULON® Fermentation Derived Cellulose A novel, naturally derived activated suspension aid for liquid laundry and other surfactant-based formulations

Presenting Author: John M. Swazey - CP Kelco

In many home and fabric care applications, there is a need to find a versatile bio-sourced product with excellent environmental credentials that can create stability of components in surfactant-based systems. The liquid laundry detergent segment is one key example where suspension of useful materials such as decorative or active beads, perfume encapsulates, etc. is desired so that enhanced cleaning can be achieved with longer lasting freshness and ease of use. However, the suspension of such key ingredients can be difficult, especially in highly concentrated surfactant systems, using any of the current available naturally derived products, and especially without adversely affecting the viscosity and pour properties of the product. CP Kelco introduces CELLULON® Fermentation Derived Cellulose (FDC) which has been developed to help meet these wide-ranging challenges. FDC is produced by the fermentation of corn-syrup based media with the bacterium, Komagataeibacter xylinus, and is a pure cellulose that is chemically identical to plant-derived cellulose. However, although chemically identical, CELLULON® FDC fibers are produced as a 3-dimensional, reticulated net-like structure and are much smaller in diameter than plant-derived cellulose. This gives a cellulose with a far higher surface area by weight ratio. This net-like structure allows the CELLULON® FDC to create a true yield value in solution at low use levels which then provides reliable suspensions of actives, decorative particles, perfume encapsulates, etc. with minimal impact on the finished product's viscosity and dispersability. Furthermore, because the FDC is completely insoluble, it does not compete for water and

therefore is highly compatible with other formulation components even in very high surfactant concentrations.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Processing

(3926) Application of Methyl Ester Sulfonate for Liquid Detergent - Improving the Physical Properties of Methyl Ester Sulfonate for the Manufacturing Process

Presenting Author: Kazuki Shimizu, MS - Lion Corporation

Addressing environmental problems such as global warming is one of corporate management's most important tasks in achieving a sustainable society. Since the 1980s, we have been developing MES, a carbon-neutral anionic surfactant made from sustainable palm oil, and have used it in powder detergent for its superior features. Furthermore, in 2012, in response to changes in the global clothing detergent market, we began selling liquid detergent formulated with MES in Malaysia. Formulating liquid detergent with MES means heating and dissolving MES flakes, so efficiently manufacturing liquid MES detergent in a range of locations, including cold places, requires improving MES solubility by developing a highly soluble, fluid MES solution. Therefore, in order to improve MES' physical properties, we examined how the ratio of C12/14 and C16/18 MES affects its physical properties. First, we looked at how this ratio impacts detergency and determined a range of ratios that improve MES solubility while maintaining detergency equivalent to C16/18 MES. Next, we verified that this ratio range produces a stable liquid MES solution at room temperature. Finally, we evaluated the improvement in manufacturability of this new MES solution.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Processing

(3727) Use of the HLD/NAC Framework in Reservoir Modeling

Presenting Author: Jeffrey Harwell, PhD - The University of Oklahoma

Simulation of enhanced oil recovery processes by surfactant flooding require the ability to predict oil/brine interfacial tension as a function of surfactant composition and concentration as well as temperature and electrolyte composition. Classically the oil/brine/surfactant phase behavior has been modeled using the empirical Hand's rule. Hand's rule requires a minimum of 5 adjustable parameters which must be determined experimentally. The HLD/NAC framework

allows more accurate prediction of the phase behavior based on a single experimental parameter, which can also be estimated from the known structure of the surfactant. Additionally, the HLD/NAC model is more computationally efficient, resulting in significant reduction in the computation resources required to perform a simulation.

Friday, January 1, 2021
Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Processing

(4152) Breaking Water-in-Crude Oil Emulsions Using a Combination of High-Throughput Material Discovery and Mechanistic Fundamental Tools

Presenting Author: Tzu-Chi Kuo - The Dow Chemical Company

Water-in-oil emulsions are commonly unavoidable and undesirable in the production, transportation, and refining of petroleum and related products. The emulsions are stabilized by a variety of surface-active compounds found in crude oil such as natural surfactants and fine mineral particles. A critical step in the processing of crude oil is to break the interfacial film formed at the oil/water interface to enable the coalescence and separation of water from oil. Demulsifiers are commonly used to promote the water removal process. However, the effectiveness of a demulsifier varies greatly due to the oil sources, water content, and processing. This presentation will describe our research efforts on breaking water-in-oil emulsions focusing on water-in-oil interfacial properties that govern emulsion stability and demulsification. High throughput techniques for rapid synthesis and screening were used to prepare demulsifiers and determine their effectiveness. Fundamental studies were also done to understand the effect of selected additives on the interfacial behaviors. Water droplet coalescence mechanisms were investigated using molecular and dissipative particle dynamics simulations, and microfluidics experiments. The modeling and empirical results show that the effectiveness of an additive is correlated inversely to the coalescence time of two droplets.

Friday, January 1, 2021

Session Time: 1:00 AM - 2:00 AM

Presentation Time: 1:00 AM - 2:00 AM

Track: Surfactants and Detergents@@@Protein and Co-Products

(3902) Critical Surfactant Requirements for Cleansing and Deposition in Shampoos

Presenting Author: Manuel Gamez-Garcia - Ashland Specialty Ingredients

The deposition of actives such as silicone, fragrance, and medicated ingredients from shampoos requires a combination of surfactants and polycations that can form a coacervate during shampoo

dilution. Experimental observations indicate that in addition to coacervate formation there are other equally important factors contributing to deposition arising from hydrodynamic, filtering, surface energy, and shear phenomena. When all these factors are considered, the analysis indicates that in order to attain deposition, while at the same time maintaining a good level of cleansing, a delicate balance between polycation and anionic surfactant properties is necessary. A discussion of cleansing and deposition mechanisms, their interaction, and final effects for various surfactants will be presented.