2013 Annual Meeting Abstracts

Surfactants and Detergents

MONDAY

AFTERNOON

S&D 1: Industrial Applications of Surfactants
Chair(s): M. Dahanayake, Rhodia, USA; P. Sharko, Shell Global Solutions Inc., USA

Single Phase Vegetable oil Microemulsion: Particle Size and Zeta Potential Characterization

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Windsor IV vegetable oil microemulsions stabilized with extended chain surfactants were characterized by particle size and zeta potential as a function of composition within the single phase region. Water-in-oil microemulsions are thermodynamically stable dispersions consisting of nanometer size droplets that produce an optically isotropic liquid. The extended chain surfactants used are linear alcohol block copolymers composed of polyoxypropylene and polyoxyethylene groups and a sulfate group at the end. The propylene oxide groups are used to extend the distance between the long carbon chain hydrophobe and ethylene oxide hydrophilic groups. This provides a more gradual transition of the hydrophobic to hydrophilic properties of the molecule. They are very tolerant of salts and are capable of producing ultra-low interfacial tension. As the water to oil ratio is increased, the emulsions undergo a phase transition from a water-in-oil (W/O) to an oil-in-water (O/W) emulsion. This results from the change in the oil to water ratio and surfactant concentration with the single phase region. Dynamic light scattering was used to measure the particle size and zeta potential as a function of dilution as they pass through this phase change.

Adsorption of Sodium Dodecyl Sulfate and Sodium Octanoate on Carbon Black and Paper Fiber in the Presence of Calcium Ions

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Deinking is an important step in recycling of waste paper and flotation is commonly used in this process. The adsorption of two anionic surfactants (sodium dodecyl sulfate, SDS, and sodium octanoate, SOC) on both a model ink (hydrophobic carbon black) and hydrophilic office paper fiber was studied. The effect of pH and the co-adsorption of calcium and surfactant on both surfaces also were investigated. SDS adsorbs on carbon black as a tail-down monolayer (hemimicelle) while on paper fiber as a head-down, head-out bilayer (admicelle). SOC forms admicelles on both carbon black and paper fiber indicating the stronger interaction of the carboxylate group with the carbon surface than the surfactant sulfate group, causing the SOC to adsorb at higher levels than SDS on carbon black. Calcium causes surfactant adsorption to increase on carbon black as it adsorbs between negatively charge surface sites and the anionic head group of the surfactant (bridging) at low surfactant levels while not enhancing surfactant adsorption on paper

fiber, explaining its activation effect in deinking processes. At high surfactant loadings calcium adsorption cab decrease (calcium exclusion effect) due to covering up of negative adsorption sites on the surface by the surfactant.

Low Voc, Biorenewable Solvents With Enhanced Degreasing Properties

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Solvents play a major role in the cleaning of hard surfaces inside and outside of the home around the globe. There is a growing concern that these materials may have an adverse impact on the environment, including health and safety issues. In recent years there have been a number of regulations passed that restrict the concentration of volatile organic carbons in select formulations. These green products often the consumer an alternative, eco-friendly option for cleaning, but the performance of these products is often inferior to other commercial offerings. Dow has developed a unique hydrophobic solvent that meets all CARB LVP criteria (non-flammable, non-VOC), is derived from 100% biorenewable materials and provides excellent degreasing performance on oily/waxy/greasy type soils on various substrates. The solvent has applicability in household and industrial formulations, and offers the formulator an opportunity to deliver improved grease cutting solvency which is a green chemistry based alternative to existing petrochemical solutions.

Powerful Tool for Developing Cost-Effective and Competitive Formulations

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Combination of Abrasion Scrub Tester (ACT) and Image Analysis (IA) is a powerful tool for developing cost-effective cleaning formulations and for supporting competitive claims. In this presentation, we will show how modified ACT is used to remove the in-house developed tenacious soiled panels. Using ACT as cleaning tool can eliminate the human application errors and serve as a more reliable automatic testing tool. The dirt on the soiled panels was removed at different extents depending on the effectiveness of the formulations. The consumer visual rating or ?blind panel test? usually can give quite an accurate result on which formulation / product performs the best. However, a more precise method to analyze the amount of dirt left on the soiled panels is needed. Work performed in our laboratories shows that Image Analysis is an accurate method that quantifies, in numbers, the dirt left on the panels. The results obtained from Image Analysis are in accord with the ?blind panel test? results. The quantified values are useful, especially when it comes to developing cost-effective products needing statistical competitive claim support.

Use of Viscoelastic Surfactant Formulations for Improving Chemical Flooding Performance

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One of the challenging tasks for chemical flooding applied in tight reservoirs is the unfavorable injectivity of polymer. Injection of viscoelastic surfactant may provide a viable approach for enhancing mobility control instead of polymer injection. The rheological properties of wormlike micelles developed with anionic surfactants were studied in natural

and mimic brines under different reservoir conditions. We investigated the effects of the surfactant concentration, the level of electrolytes, reservoir temperatures, and various co-surfactants on the rheological properties. We observed markedly increase of the viscosity (one order of magnitude) at reservoir temperature of 50oC by introducing trace amount of the selected co-surfactants. The newly developed viscoelastic system is expected to offer better sweep efficiency in low permeability reservoirs as compared to classical EOR polymers. The injected wormlike micelles would change their shape as they pass through tiny pore-throats in reservoir rock where the shear rate is high and then reform after they reach to large open region. Core flood results prove that wormlike micelles would not plug the core unlike the high molecular weight polymers. Different surfactant and polymer combinations were tested for achieving synergism while increasing viscosity in situ and decreasing the amounts of surfactant required for oil recovery.

High Throughput Development of Formulation to Face new Constraints

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Chemists and formulators have to face evolving constraints to provide well adapted solutions to consumers. Sourcing of the raw materials to prepare a surfactant (availability and/or bio-sourcing) and regulatory issues currently are strong drivers toward alternative formulations. In surfactant formulations, the spectrum of eligible molecules in different conditions (concentration, pH, salinity, temperature?) is broad. Therefore, the number of solutions to evaluate can be unreachable in a classical way of formulating. Addressing these challenges requires a lot of testing of new formulae in a short time. We propose to use high throughput (HTP) technologies to quickly qualify and evaluate a large number of formulations. To that aim we develop both robotics and a micro- or milli-fluidics based tool that can truly leverage innovation in that direction, allowing an increase in research productivity (decrease in needed volumes, shorter evaluation time). Robotics and fluidics are complimentary approaches (multi-batch, continuous) that both will be presented. It will be shown how they can be useful to increase productivity of research. Our purpose will be illustrated with some applied examples of surfactants formulations. We will show how the efficiency of HTP methods can help providing alternative ingredients for formulations that are better adapted to new constraints.

PROTON-INDUCED EMULSION RUPTURE LEADING TO MULTI-LAMELLAR MACRO-EMULSION.

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Salt-induced changes in emulsion morphology including multi-lamellar formation and emulsion size enlargement were studied its underlying mechanism. With the addition of small amount of acid, multi-lamellar layered macro emulsion droplets are generated simultaneously and a clear 'maltese crosses' was detected by plane polarized microscope. We consider this as a result of structural change on surfactants (stearic acid) caused by catalytic amount of proton influx which is accompanied by a chained deformation of emulsion morphology. Fattyl acids with different chain length were tested. Oil polarity didn?t affect the system. A wide range of surfactants was screened and cetearyl alcohol and coco glucoside was selected as the best emulsifier that shows macrolamellar formation. This study was motivated by the fact that long chain quaternary ammonium salts with sodium salicylate (NaSal) show the phenomenon of viscosity rise at very low ionic strengths and then viscosity drops off drastically.

TUESDAY

MORNING

S&D 2: Surfactants in Energy
Chair(s): U. Weerasooriya, University of Texas, USA; B. Shiau, University of Oklahoma, USA

Synthesis and Surface Activity of a Class of Novel Triazine Carboxyl Betaine Surfactants Derived From S-triazine

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Six series of asymmetric triazine betaine surfactants (BC10-8, BC12-8, BC14-8, BC12-10, BC14-10, BC14-12) have been designed and synthesized through four-step reaction. Their structures were confirmed by IR, NMR and mass spectrometry. Surface activity of these surfactants was tested and it was found that surfactants BC10-8, BC12-8, BC14-8, BC12-10 exhibited superior surface activity as 25.4mN/m, 23.2mN/m, 22.3mN/m, 24.1mN/m, 30.2mN/m and 34.0mN/m, respectively. While interacting with alkane from hexane to hexadecane, these surfactants showed a good ability to reduce the interfacial tension to 10-2 mN/m, which is a beneficial exploration for these surfactants and crude oil.

Performance Improvement Trends to Attain Ultralow Interfacial Tension With Surfactant Formulation in Enhanced oil Recovery

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Enhanced oil recovery by surfactant flooding is a candidate to maintain the required oil recovery in the next decades. The low price of petroleum in the 1980-2005 period has considerable reduced the technical work in EOR but more fundamental research has provided a huge amount of information on the relationship between the formulation and the ultralow tension attained at te so-called optimum. The present review shows that there are many ways to increase the actual performance since Winsor's premises back in the 1950's, but also remarks the trends are often associated with limits which have to be either further displaced or compensated. Formulation optimization is shown to depend on surfactant molecule design with a conflict between molecular size and precipitation, on intermolecular mixtures with a conflict between better interfacial behavior and lost species into the bulk phases, and on intramolecular mixtures which is still an innovative area. Currently proposed best formulas are matching a combination of all these trends with a large variety of alternatives.

Synthesis and Application of High Molecular Weight Sulfonates.

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This presentation will discuss the synthesis of high molecular weight arylalkyl sulfonic acids and their salts. These surfactants are derived from a the reaction product of alpha olefin sulfonic acids with an aromatic and subsequent addition of an olefin, an olefin sulfonic acid, an unsaturated fatty acid, or an unsaturated fatty acid alkoxylate or and carboxylated unsaturated fatty acid alkoxylate. Sulfonic acids having molecular weights from about 400 to over 800

can be easily manufactured using both petrochemical and natural feedstocks. The reaction rates of alkylation are extremely fast leading themselves to a continuous process. The starting arylalkyl sulfonic acid is an extremely powerful alkylation catalyst and can be used in place of HF or AlCl3 for alkylation processes. Examples of the application of high molecular weight sulfonates to produce ultra-low interfacial tensions for recovering petroleum will be presented.

New Developments in Chemical EOR

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New Chemical EOR formulations have been developed that can withstand harsh reservoir conditions. Such harsh conditions include very high temperatures, high salinity, and high hardness ions. Laboratory phase behavior experiments were employed to develop surfactant formulations and their efficasy were verified by coreflood experiments. The new formulations were designed with special emphasis on their commercial viability including cost effectiveness.

Surfactant Enhanced Oil Recovery from Naturally Fractured Reservoirs

J. Lu[(1)], A. Goudarzi[(2)], P. Chen[(3)], D. Kim[(4)], C. Britton[(5)], M. Delshad[(6)], K. Mohanty[(7)], U. Weerasooriya[(8)], G. Pope[(9)]
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Large volumes of oil remain in naturally fractured carbonate oil reservoirs and water floods are often very inefficient because many of these reservoirs are mixed-wet or oil-wet as well as extremely heterogeneous. Naturally fractured reservoirs are challenging targets for chemical flooding because they typically have a high permeability contrast between the fractures and the matrix with low to extremely low matrix permeability. In addition, some of the world?s largest oil reservoirs are fractured carbonates with high reservoir temperature and high salinity formation brine and some of them also have low API gravity oils, which also increases the difficulty of recovering the oil. We have developed a stable surfactant that shows promising results even when all of these conditions are present at the same time. Both static and dynamic imbibition experiments were done using a fractured carbonate core. These results were interpreted using a mechanistic chemical reservoir simulator.

Designing Surfactant Formulations for Enhanced oil Recovery by Using the Hydrophilic-lipophilic Difference Concept

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The hydrophilic-lipophilic difference (HLD) equation has been used as a designing tool in formulating potential surfactant candidates for enhanced oil recovery for mature fields. The critical reservoir and fluid properties (the brine salinity (S*); the equivalent alkane carbon number (EACN) of the crude oil; a surfactant head group parameter (K); the characteristic curvature of the surfactant molecule (Cc); and functions for co-surfactant or alcohol, f(A), and temperature, ?T?T) are used in the HLD equation to predict the optimal microemulsion formulation under different reservoir conditions. The surfactant ratio is scanned around the HLD prediction to experimentally determine the optimal surfactant ratio based upon interfacial tension measurements. In this study, both surfactant system with and without alcohol are investigated. A comparison between the HLD prediction and experimentally determined optimal surfactant formulation for several target oil fields will be presented and discussed. The results of oil mobilization in one dimensional sand pack and core flood tests will also be presented to demonstrate the performance of the designed chemical formulation suitable for further field single-well tests.

Solubilization Capacity and Emission Characteristics of Vegetable Oil-based Microemulsion Biofuel

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Vegetable oil-based microemulsion biofuels are being considered not only to reduce the viscosity of vegetable oil but also to overcome the immiscibility of polar phase and oil. Surfactant solubilization capacity is an important parameter utilized in many industrial applications to quantity the ability of surfactants to enhance ?miscibility?. For reverse micellar microemulsion, this parameter indicates the capacity of a polar phase to be solubilized in oil phase, which depends on the structures and the interaction of the polar phase. From our previous study, a microemulsion fuel of vegetable oil was formulated by using the nonionic surfactant with ethanol as a polar phase. However, the effect of structures of polar phase on the solubilization capacity has yet to be evaluated. Therefore, the objective of this study is to determine the effect of structures of polar phase on the solubilization capacity of polar phase in oil microemulsion. In addition, the emission characteristics of the selected microemulsion fuel formulation will be studied to compare with those of No.2 diesel.

Palm oil Microemulsion-based Biofuel: Environmental Impact Assessment

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The issues relating to global warming, energy prices, and the uncertainty of future fuel supplies, have created a strong interest in the alternative renewable transportation fuels. Palm oil reverse micelle microemulsion, which can be formulated from the renewable resources at low-energy input without waste generation, has been considered as one of the promising alternative for transportation fuel. The objective of this research is to quantify and verify the life-cycle environmental impacts including greenhouse gas and acidification effects of microemulsion-based biofuel (MB50), formulated from the mixture of Methyl oleate/1-Octanol (mole ratio of 1:8), ethanol (20 vol%), and palm oil/diesel blend (50 vol%). The system boundary started from raw material production to delivery to the vehicle tank for the evaluation of the well-to-wheel (WTW) analysis. Moreover, environmental impacts of MB50 production were compared to those of comparative fuels; biodiesel blend (B50, 50 vol% of neat biodiesel + 50 vol% of diesel) and diesel. From the environmental point of view, microemulsion-based biofuel appears attractive since it has significantly less environmental impacts in comparison to biodiesel and diesel. Thus, this study can be considered as an opportunity for further research and evaluation of the available options for a sustainable transportation system.

Designing Surfactant-only Formulations for a High Salinity and Tight Reservoirs

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This study explored the use of surfactant-only system for EOR application at a high salinity (164,000 ppm) and tight formation (permeability of 17 millidarcy). Several low IFT surfactant formulations were successfully developed under target reservoir conditions. Instead of polymer injection, wormlike micelle system was applied to achieve elevated viscosity at high brine condition enabling better mobility control during the chemical flooding. The newly developed surfactant and wormlike micelles formulations were further verified in 1-D packed column using Berea core, site-specific crude oil and brine to fine tune the injection strategies for field single-well tests. Among the promising candidates, a binary surfactant mixture of propoxylated/ethoxylated alcohol sulfate and ethoxylated alcohol sulfate (0.325 wt% total) offered an exceptional performance (IFT of 0.006 mN/m). Introducing wormlike micelles of anionic ethoxylated alcohol sulfate (1 wt%) combined with a hydrophilic linker produced the desired viscosity of 45 cp at reservoir temperature of 36 °C. The resulting surfactant and wormlike micelles solutions remain stable over extended period (> one month). Injecting 0.1 PV wormlike micelles chasing with 1.5 PV surfactant-only slug achieved markedly improvement of oil recovery in the packed column.

S&D 2.1: General Surfactants

Chair(s): R. Panandiker, Procter & Gamble Co., USA; D. Murphy, Stepan Co., USA

Novel Surface Modifying Technology for Enhanced Hard Surface Cleaning Experience

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Home care hard surface cleaners contain surfactants and performance ingredients which are used to clean dirt, stains and grease from surfaces. Consumers desire cleaning products which refresh and clean the surface, enhancing the overall cleaning experience. Lubrizol introduces a novel surface modifying technology specially designed to impart shine, provide stain protection and water repellency to hard surfaces during the cleaning process, providing a strong visual impact. Surfaces are often dulled by residual surfactants and/or normal wear. Current commercial products that restore shine often suffer from poor water and stain resistance. Application and performance testing results of the new technology will be discussed. The performance versatility allows for its use in a wide range of general cleaning formulations for a wide variety of surfaces such as wood, ceramic, laminate, granite, concrete and stainless steel. Surface refurbishing performance is demonstrated for premium floor cleaners, and polishes. This technology provides one step cleaning options in formulating innovative systems for surface care.

Encouraging the Adoption of Green Cleaning by Preserving the Performance of Peroxygen Cleaners Over the Long Term.

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The market acceptance of green cleaners historically has suffered from several challenges, the chief one being a lack or loss of cleaning performance. With the proliferation of peroxygen-based cleaners in the market, the performance focus for these products has been on oxidizer stability. Other issues that plague these formulations while in storage such as loss of pH, onset of cloudiness, and loss of cleaning performance have all been ignored. The goal of this presentation is to propose a cause of the problem, suggest a solution to this problem, and then present data that shows the problem can be corrected. Data collected includes pH, turbidity, hydrogen peroxide assay, reverse phase HPLC, C13 NMR, and ASTM D4488 cleaning efficiency. Under accelerated aging conditions it has been found that a control sample shows a drop in pH (over 2.5 units), along with the onset of turbidity and loss of cleaning performance. An inhibited sample aged in the same fashion has little drop in pH, remains clear and continues to clean. Preserving cleaning performance by protecting the surfactant from attack through the use of this chemistry also provides an increase in hydrogen peroxide stability. These inhibiting materials are naturally occurring and commonly found in health supplements routinely consumed by the general public.

Next Generation Hybrid Polymers - a More Sustainable Solution

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AkzoNobel has developed a new, biodegradable biopolymer technology for the Fabric and Cleaning marketplace. Based upon the combination of selected polysaccharides and synthetic monomers, the Hybrid Polymers of this technology biodegrade in the environment, offer a preferable carbon footprint, and are effective in replacing synthetic polymers in formulations such as automatic dishwash and laundry detergents. This 2nd Generation technology provides a sustainable and cost effective alternative to existing synthetic options. This paper will provide insight on the latest developments with AkzoNobel Surface Chemistry?s readily biodegradable Hybrid Polymer Technology. Specifically, the performance of these polymers in automatic dishwash and laundry detergents, and their positive environmental aspects will be reviewed, including lifecycle analysis.

Sulfonation Reaction Analysis of Converting Fatty Acid Methyl Ester to Fatty Acid Methyl Ester Sulfonate (MES).

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Fatty acid methyl ester sulfonate (MES), an anionic surfactant suitable as a laundry detergent, is produced commercially by the direct sulfonation of fatty acid methyl ester (ME) with SO3. However, an intense coloration occurs during the sulfonation process. The sulfonation of ME was performed through the addition of SO3 (SO3/ME molar ratio = 0.8?1.2) for 1?4 hr at 80 °C and subsequent aging for 1 hr at 80 °C. Even when the amount of unsaturated bonds in ME was reduced to give an iodine value (IV) of less than 0.01, coloration occurred during the sulfonation, making the product unsuitable for commercial use. So we performed quantitative analyses of unsaturated bonds, SO2 and MES in the reaction mixture and for the gaseous product during the reaction. As a result, we found that equimolar amounts of the olefinic unit and SO2 were formed, the rate profiles of the formation of MES and SO2 correlated well with each other, and the color-intensity of the reaction mixture increased by increasing their amounts during the reaction. From these observations, we concluded that the coloration of the reaction mixture was caused by oxidation of the alkyl chain with SO3 during the release of SO3 from the 1:2 adduct of ME and SO3, a key intermediate in the formation of MES from ME in the sulfonation process.

Organomodified Silicones in Household Care

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Silicones have multiple benefits, but the biggest limitation is in compatibility with other chemicals. Modification of silicones with organic moieties can help overcome this limitation. Incorporating various organic functional groups can result in unique properties and structures like silicone quaternaries, betaines, surfactants, waxes, etc. These modifications significantly broaden their application areas and can improve their environmental impact, even some cases reaching ?readily biodegradable? status. The detailed chemistry and application benefits will be discussed in the presentation.

Alternative Chemistry for Polyacrylate Replacement in Sustainable Liquid Laundry Detergents

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[(1)]Thermphos - Dequest, United States of America [(2)]Thermphos - Dequest, United States of America [(3)]Thermphos - Dequest, United States of America

The global demand for liquid laundry detergents is ever increasing along with the cleaning performance expectations. Today?s detergents must work well in difficult conditions such as cold water wash without the use of traditional chemistries such as phosphates. These demands include higher rates of concentration, the need for more effective and highly soluble ingredients, stable enzyme systems effective at low temperature, and powerful anti-redeposition agents. To meet these demands, Dequest developed a new product based on a vegetable polymer co-builder system. The product was designed to improve the performance of today?s high performing detergents while improving their sustainability profile. In particular under low temperature washing conditions, Dequest®?s SPE 1202 shows improved contributions to both primary and secondary washing performance versus polyacrylates mainly due to its high water solubility, very good dispersing (anti-redeposition) properties and its excellent compatibility with calcium dependant enzymes. Current laboratory results show that it is a cost-effective alternative to acrylic polymers in liquid detergents under today?s lower temperature washing conditions.

Novel new Surfactant Molecules With Sulfoxide Headgroups

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[(1)]University of Oklahoma, United States of America [(2)]University of Oklahoma, United States of America [(3)]University of Oklahoma, United States of America [(4)]Novus International, United States of America [(5)]Novus International, United States of America

This talk discusses new and novel nonionic surfactants containing a sulfoxide hydrophilic moiety within the main chain. Although not new, the sulfoxide headgroup has been very rarely studied and has the advantage over more common ethylene oxide headgroups as not having a cloud point. This talk will discuss in detail the structure and physical chemistry of these molecules. Surface tension, critical micelle concentration, water solubility, Draves Wetting test and Ross-Miles foam test results will be reported, and compared to other similarly structured surfactants. In general, these molecules tend to have good wetting properties, have relatively low cmcs, extremely low surface tensions (for a hydrocarbon-based surfactant) and tend to make significant, but unstable foams.

Synergies of Long-chain Alkyl Amidinium Bicarbonates With Anionic Surfactants

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Long-chain alkyl amidinium bicarbonates, as a series of novel cationic surfactants, have been attracting a lot of attention due to their excellent properties (especially the switchablity with CO2) since it was reported in 2006. Cationic and anionic surfactants have strong interaction and form complexes, resulting in many changes in their properties, can generate significant synergies, which make the complex superior performance to a single surfactant. Therefore, four N?-alkyl- N,N-dimethylacetamidines (decyl, dodecyl, tetradecyl, hexadecyl) were synthesized and selected as cationic surfactants. Two commercial anionic surfactants, sodium dodecyl benzene sulfonate (SDBS) and sodium dodecyl sulfonate (SAS), were selected as anionic surfactants. The complex systems of these cationic and anionic surfactants show more excellent surface activity than that of single anionic or cationic surfactant, reflecting that the CMC of mixed surfactants was 2 orders of magnitude lower than that of single surfactant in different mole ratio, and the surface tension is also lower. The interaction parameters between surfactant molecules in micelles of mixed system (?), which are calculated by CMC of anionic, cationic and the complex, indicate the existence of an attractive interaction between these cationic/anionic systems.

AFTERNOON

S&D 3: Consumer and Cleaning Applications
Chair(s): B. Lin, Henkel, USA; T. Graham, Sun Products Corp., USA

Synergistic Combination of Extended-surfactants and Biorenewable Surfactants for Cold Temperature Detergency of Vegetable Oils and Fats

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The goal of this work is to investigate the detergency performance of mixtures containing extended-surfactants, biosurfactants and bio-renewables surfactants at 10 and 25 degree Celsius with vegetable oils and fats. Three types of vegetable oils and fats were studied, including canola oil (liquid oil), jojoba oil (wax) and coconut oil (solid fat). Detergency of vegetable oils and fats is challenging at best due to their highly hydrophobic property and crystalline structure of fats. Extended-surfactants in the past have shown superior detergency performance (>90%) with canola, but required very high salinity (>8%). In this work, we showed that mixtures of extended-surfactants with lipophilic biosurfactants (i.e. sophorolipids) or bio-renewable surfactants (i.e. sorbitan fatty acid esters) have synergistic effect in the detergency performance, while decreasing the required salinity concentration appreciably. The chemical structure of lipophilic surfactants is critical in the detergency of fats. Branching lipophilic surfactants disrupt the crystalline structure of fats; thereby improving the detergency.

Visualizing Cleaning Process Real Time ---novel Hard-surface Cleaning Surfactant System That Clean Quickly

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Recent market trend in hard-surface cleaning (HSC) is an increasing focus on efficiency and ease of cleaning (e.g. good cleansing with less soaking time and minimum reps of gentle wipes). Surfactants used in this type of HSC product formulations need to quickly supply chemical energy to the cleaning process and leave no residue. To address this need we have developed a new line of C9-based nonionic surfactants (Patent Case TH 4211) that deliver superior cleaning performance at short contact times. In this talk, we present the test results of our new nonionic surfactants using a HSC performance test method with real-time video monitoring that is capable of resolving cleaning performance in stroke-by-stroke detail. Using this new method we can demonstrate that our new surfactant systems deliver superior cleaning in a simulated spray-and-wipe application.

The Realisation of the Impossible: the Stabilisation of Reactive Benefit Agents in Laundry Liquid Formulation and Their Efficient Release in Wash

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In recent years the use of liquid laundry detergents has grown enormously as households have embraced the convenience that liquids provide. However, there are important performance differences in the cleaning efficacy of liquids compared to powders and in order to close this gap the industry has been seeking new technical solutions. Liquids, for example, cannot be formulated with the inclusion of reactive benefit agents because such benefit agents will react unfavourably with the aqueous formulation ingredients. This presentation will describe a new approach developed by Revolymer?s scientists to stabilise reactive benefit agents in liquid laundry products. However, stabilisation is only half the story ? the presentation will also describe the how stimuli responsive materials may be used to ?sense? their environment leading to the efficient release of the benefit agent when the product is used in the wash.

The Foaming Control Technology for the Rinsing Improvement in Laundry Detergent.

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In recent years multi-functional laundry detergents have been attracting a lot of attention due to consumer?s expectation beyond cleanliness. The cationic surfactants are the typical functional ingredients that add an anti-bacterial effect, softness and maintain fragrance on clothes after rinsing. Generally cationic surfactants make the anion/cation complex under the co-existence of anionic surfactants in water solution. Because of stabilization of foam film by these complexes, detergent solution shows a rich foam and poor rinsability. The rinsability is a very important property that enables the reduction of water consumption during the laundry process. Through our evaluation for various agents, the solvent of ester origin which had the dramatic de-foaming effect was found. This is a new de-foaming approach which is neither silicone nor low-foaming surfactant.

Real Time Study of Detergent Ingredient Action: stain Removal and Adsorption of Benefit Agents

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Today?s laundry detergents are complex mixtures of various surface active ingredients. Often they combine stain removal action with the adsorption of benefit agents for textile care. In order to optimize detergent performance and to understand the influence of individual ingredients, it is of interest to investigate in detail interaction of such materials with each other and with textile surfaces. The quartz crystal microbalance (QCM-D) technique is perfectly suited for this challenging task because it opens up the possibility of monitoring processes on a specific surface in real time. Adsorption as well as desorption processes are accessible, and various factors influencing the detergent action are easy to control, e.g. temperature. The QCM-D technique was used in this study to investigate the removal of skin fat. Thin fat films were deposited on the surface of a QCM sensor. A two step mechanism of initial swelling of the fat film followed by fat removal was monitored in real time. Furthermore, polymer adsorption on cellulose fibers was investigated by using cellulose model surfaces attached to the sensor surface. The impact of ionic strength, surfactants and the adsorbing polymer could be clearly shown.

Novel Anti-microbial Benefits for Lactic Acid

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In recent years there has been substantial growth in household products with anti-microbial claims. This growth has been generated by growing consumer concerns over health and hygiene issues triggered, for example, by fears of deadly viruses and bacteria such as the Swine Flu virus and EHEC bacteria. Claims such as "kills up to 99.9% of germs" are increasingly the norm, especially in the surface care and toilet care area. Lactic acid can be used as a biobased anti-microbial agent. The anti-bacterial benefits of lactic acid are widely known. It is therefore already applied as an active ingredient in a wide range of cleaning and disinfecting products in home care, industrial and institutional applications. Besides the anti-bacterial benefits, lactic acid can now also bring anti-virus benefits to detergent formulations. Novel formulation developments and anti-microbial efficacy testing have revealed good anti-virus performance against a range of enveloped viruses. The combination of anti-bacterial and anti-virus action into one single ingredient makes lactic acid a versatile ingredient with a wide range of anti-microbial efficacy. Lactic acid has GRAS status and is therefore safe for food contact. It is a natural and biobased ingredient, which is readily biodegradable and non-toxic to the environment and humans. It shows no skin sensitization, nor resistance build-up. Therefore lactic acid offers a safe alternative to many traditional biocides.

Monoglyceride Removal From Fabrics Under Microemulsion-base Formulation

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The aim of this research was to apply a microemulsion ? based formulation for the removal of solid oily soil in laundry detergency. To form middle phase microemulsion (winsor type III), two different surfactants were used: branched alcohol propoxylate sulfate sodium salt (C12,13-(PO)4-SO4Na), an ionic surfactant and sodium mono and dimethyl naphthalene sulfonate (SMDNS), a hydrophilic linker. Methyl palmitate or palmitic acid methyl ester was selected as a model of solid oily soil and two types of fabrics were studied: pure polyester and pure cotton. The detergency experiments were carried out in a Terg-O-Tometer at different total surfactant concentrations, salinity and temperatures (10 to 50?C) to cover both lower and higher than the melting point of the studied oil (30?C). Furthermore, the re-deposition of removed soils was also investigated. From the preliminary results, a mixed surfactant

system of 86 parts C12,13-(PO)4-SO4Na and 14 parts SMDNS of the optimum salinity at 5.3% was used as the selected formulation on detergency performance. The microemulsion-based formulation reach plateau in detergency at 0.35% total surfactant concentration with efficiency 70% oil removal at above oil?s melting point and soil re-deposition performance decreased when increasing total surfactant concentration for both types of fabrics. Additionally, the cotton fabric showed the highest detergency efficiency while the polyester gave the lowest performance.

Enhancing Whiteness Through Enzymes.

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Enzymes can provide natural whiteness and deliver deep cleaning helping reformulate detergents with lower levels of ingredients, including optical brighteners. Whiteness is an important cleaning parameter that can have different meanings in different regions. Loss of whiteness can be e.g. due to greying, yellowing, color transfer, or removal of optical brightener agents. Whiteness reduction due to greying and/or lack of soil removal can be addressed with enzymes. Reduced whiteness due to reduction of ingredients can also be addressed with an enzymatic system, e.g. enzymes can help optimize the use of optical brighteners and improve the environmental and sustainability profile of the detergent. Optical brighteners adsorb to the fabrics during wash and mainly impart a whiter and brighter look to the fabrics making them look cleaner than what they truly are. Enzymes contribute even further to the deep cleaning process that results in the fabric whiteness and care. Through the use of readily biodegradable, efficient enzymes, detergents can still be high performing and tough on dirt and stains. Examples will show how customized enzyme solutions help reduce the level of optical brightener in detergents without compromising performance contributing to whiteness, and help maintain it even when optical brightener level is reduced. This means that detergent manufacturers can potentially replace part of the chemicals used in their detergents with powerful, more environmentally-friendly enzymes to give consumers a more eco-efficient and high-performing detergent. This will assist detergent manufacturers in formulating laundry solutions that indeed clean cotton apparel with natural whiteness.

Hydrogen Peroxide for Green Cleaning Applications

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Hydrogen peroxide, which is considered a green chemical because of its decomposition to water and oxygen, has found increased interest for a variety of cleaning applications. Hydrogen peroxide is an effective oxidizer and color-safe bleach for stain removal, and also functions as a broad-spectrum microbiocide for disinfection and sanitization purposes. This paper presents recent research exploring the benefits of hydrogen peroxide towards cleaning & biocidal performance, and also considers factors influencing compatibility and stabilization of hydrogen peroxide with other common components in cleaning formulations.

S&D 3.1a: Rheology and Characterization in Structured Surfactant Solutions, Including Solutions with Ionic and/or Organic Liquids
Chair(s): B. Grady, University of Oklahoma, USA; N. Komesvarakul, Sun Products Corp., USA

Surfactant-activated Microgels

K. Chari[(1)], R. Hsu[(2)], P. Bhargava[(3)], B. Figura[(4)], Y. Wayne[(5)], J. Park[(6)], T. Clifford[(7)], M. Kadir[(8)], G. Benedikt[(9)]

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Microgels are used as rheology modifiers in a broad range of applications. Commercial microgels typically comprise chemically crosslinked polymers with a pH-responsive moiety. Free-flowing dispersions of these polymers may be mixed with other ingredients in a formulation and then neutralized. Upon neutralization, the polymers swell to form a close-packed network of swollen crosslinked particles imparting rheological features such as yield stress, viscosity, shear-thinning and optical clarity. Well-known examples of pH-responsive microgel rheology modifiers are crosslinked polyacrylic acid polymers and alkali-swellable emulsion (ASE) polymers. However, pH-responsive microgels suffer from the disadvantage that desired properties are obtained only over a limited span of pH and significant changes in properties are observed in the range of pH values close to the pKa. Here we describe a new class of nonionic (non-polyelectrolyte) microgels comprising crosslinked amphiphilic copolymers of alkyl acrylates and hydroxyalkyl esters that are activated by surfactant instead of pH. We discuss the mechanism of action of these materials as a combination of swelling of individual polymer particles by surfactant micelles and surfactant-mediated interaction of the swollen microgels using dynamic light scattering (DLS), dynamic rheology and 1H NMR. In contrast to polyelectrolyte microgels, we demonstrate uniform properties over a broad pH range.

CANCELLED - Development of nano-structured products by self-assembly of surfactants

D. Bajpai[(1)], V. Tyagi[(2)]

[(1)]NONE, India [(2)]Harcourt Butler Technological Institute, India

Formulation and Rheological Properties of Structured Surfactant Systems

g. smith[(1)]

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Structured surfactant formulations (SSF) have been used for the last 30 years in a variety of detergent and personal care cleaning applications. Structured surfactant systems are most commonly based on lamellar phase surfactant solutions which can be distinguished by various experimental techniques such as optical microscopy, small angle x-ray scattering (SAXS) and cryogenic TEM. SSF technology is capable of suspending insoluble materials including solids, liquids or gases. The formulation of three different types of structured systems has been investigated. Conventional structured surfactant technology relies on forcing dissolved surfactant into multi-walled lamellar droplets using electrolyte. The surfactant droplets form a packed array with a yield stress capable of suspending insoluble particles. Commonly used insolubles include STPP as a builder for laundry formulations and calcium carbonate as an abrasive material for hard surface cleaning. Sugar-based structured surfactant systems (S4) relies on forcing surfactant dissolved in a concentrated sugar solution into lamellar droplets using electrolyte and terpene molecules. S4 systems are optically clear but beautifully birefringent under polarized light. S4 can be used as a delivery vehicle to suspend encapsulated actives in an aqueous system. Anhydrous structured liquids consist of reversed lamellar droplets

suspended in a liquid nonionic surfactant. Anhydrous systems have a yield stress which can be used to suspend water sensitive insoluble like bleach or soda ash for cleaning applications. Conductivity and oscillatory rheology have been used to formulate stable systems with no syneresis or sedimentation overtime.

Polymer - Surfactant Interactions

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Identification and characterization of the impact of polymeric rheology modifiers in surfactant systems will be examined.

The effect of surfactants on the rheology of organogels and hydrogels

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In this presentation we will describe the role that surfactant play in the formation of sterol organogels, block copolymer hydrogels and gellan gum hydrogels. In the case of sterol organogels, the changes in elastic modulus, and gel strength (measured via texture analyzer) is highly dependent on the concentration of the sterol gelling agent. In that case, the presence of the surfactant plays a minor role, and in some cases it can be detrimental due to the potential entrainment of water when the organogel is immersed in an aqueous environment. For the case of hydrogels, hydrophilic surfactants, depending on the interaction with the gelling agent, can prevent the formation of the gel and in some cases they can increase the strength of the gel. We will discuss these surfactant-gelling agent interactions in light of experimental evidence obtained from small angle x-ray scattering (SAXS), calorimetry and surface tension measurements.

S&D 3.1b: Advances in Surfactant-Based Complex Fluids

Chair(s): E. Szekeres, Clorox Services Co., USA; A. Teneja, BASF,; P. Varanasi, BASF,

Predicting Microemulsion Thermodynamics Using Unifac and Curvature Models

A. Boza[(1)], E. Acosta[(2)]
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Microemulsions are thermodynamically stable systems that contain oil and/or water nano-domains stabilized by surfactants adsorbed at the oil-water interface. Microemulsions are of great interest in various applications including enhanced oil recovery, environmental remediation, pharmaceutics, cosmetics and others. The most accurate methods for predicting the phase behavior of microemulsions involve the use of semi-empirical curvature models. Recent literature connects this curvature term to surfactant partition between oil and water. In this research, the original UNIFAC model has been used to evaluate the partitioning coefficient of ethoxylated alkylphenol surfactants in microemulsion systems as well as the effect of temperature on the phase behavior of these systems. To obtain an appropriate representation of the systems mentioned before, new interaction parameters have been included to the original UNIFAC model (Fredenslund and others 1975). Additionally, modification of the temperature dependency of the interaction parameters is proposed to overcome problems of the original UNIFAC model for ethoxylated surfactant

systems. Initial studies show that predictions of the original UNIFAC with adequate inclusion and modification of the temperature dependence of the parameters provide the adequate trends of the systems under study.

Van der Waals Free Energy Model for the Solubilisation of oil in Micelles

A. Boza[(1)], E. Acosta[(2)]
[(1)]University of Toronto, Canada [(2)]University of Toronto, Canada

Winsor proposed to consider the ratio between surfactant-water and surfactant-oil interactions as a qualitative approach to understand the phase behavior of microemulsions. While most agree that this ratio is useful as a theoretical framework, it has not been used in a quantitative form because of the difficulty in calculating these interactions. This work presents a thermodynamic model that estimates the lipophilic ? van der Waals (VdW)-interactions between oil-oil, surfactant-surfactant, and surfactant-oil that determine the solubilisation of oil in micelles. To this end, two models for the integration of the VDW interactions are introduced, one sphere-shell to account for oil-oil and surfactant-oil interactions, and a cone-shell model to account for surfactant-surfactant interactions. Both models were derived using the microscopic approach of Hamaker and the resulting integrals were validated by comparing their prediction to selected physical properties of linear alkanes. The sphere-shell model predicts, with reasonable accuracy, the surface tension of alkanes at room temperature and reproduces the near zero surface tension values that are obtained close to the critical point. The cone-shell model, in association with the sphere-shell model, predicts the cohesive energy of different alkanes, showing close agreement with the experimental data. The combination of the two models produced a model that calculates the free energy changes associated with the solubilization of oils in micelles starting from oil and oil-free micelles. This free energy model predicts trends in oil solubilisation that are consistent with those obtained via experiments and via the semiempirical Hydrophilic Lipophilic Difference-Net Average Curvature (HLD-NAC) model.

Prediction of emulsion formation and stability with the HLD-NAC model

E. Acosta[(1)], S. Kiran[(2)]
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The HLD-NAC model uses the hydrophilic-lipophilic difference (HLD) scale to quantify the approach to the phase inversion point of surfactant-oil-water (SOW) systems. The net-average curvature (NAC) makes use of the HLD to predict the composition, density, viscosity, and interfacial tension of SOW systems. This presentation will describe how these predicted properties, along with simple fluid mechanics considerations, can be used to predict the formation of emulsions around the phase inversion point. The second part of this presentation will describe a collision-coalescence-separation (CCS) model that predicts the separation time for emulsions around the phase inversion point. The implications of these predictions on the formulation of stable emulsions and the selection of the appropriate emulsifiers will be discussed.

WEDNESDAY

MORNING

BIO 4/S&D 4: Biobased Surfactants, Detergents and Oleochemicals

Chair(s): G. Smith, Huntsman Performance Products, USA; D. Hayes, University of Tennessee, USA; D. Solaiman, USDA, ARS, ERRC, USA

Vegetable Oil Based Surfactants: Physical Chemistry and Performance Properties

G. Smith[(1)]
[(1)]Huntsman Corporation, United States of America

Vegetable Oil Based Surfactants: Physical Chemistry and Performance Properties Modern surfactants are based on either naturally derived or synthetic feedstocks. Natural surfactants are typically based on alcohols derived from coconut or palm kernel oil whereas synthetic surfactants are based on ethylene derived from gas, oil and coal. Synthetic surfactants are not based on renewable feeds and in recent years there has been increased demand for more sustainable alternatives. While natural alcohol based surfactants based on coconut or palm kernel are more sustainable, there has been increased concern about destruction of the rain forest and resulting loss of biodiversity. This presentation will discuss the physical chemical properties of surfactants based on vegetable oils like soy and canola as low cost, locally grown alternatives to conventional natural and synthetic based surfactants. A series of vegetable oil based surfactants were prepared by reacting different natural oils like soy and canola with different polyols. Depending on the polyol employed, different types of surfactants can be prepared. Reacting ethoxylated glycerin with the triglyceride gives vegetable oil ethoxylates (VOE). The properties of vegetable oil derived surfactants have been compared to more conventional natural alcohol ethoxylates (AE). In general, vegetable oil surfactants have a lower CMC, cloud point and foam potential than AEs due to the longer alkyl chain length. Surface and interfacial tension depend on the alkyl chain distribution and the degree of polymerization on the polyol. Vegetable oil derived surfactants show good detergency in single surfactant and multi-component systems.

Biobased Surfactants: Overview and New Directions

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Biobased surfactants continue to gain popularity due to concerns for sustainability and the long-term availability of petrochemical feedstocks. In this presentation, market information and overall trends for biobased surfactants will be reviewed, with major commercially available biobased surfactants identified. New biobased surfactants under development, as described in recent Journal of Surfactants and Detergents publications, will be described.

Sophorolipids as Antimicrobials and as Composite Additives for Phenotypic Alteration of Polyhydroxyalkanoate Film Surfaces

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Sophorolipids are microbially-based glycolipids that are synthesized in high yields from certain species of Candida yeasts. Because of their chemical structure, which normally consists of sophorose (2?-O-beta-glucopyranosyl-beta-D-glucopyranose) and a C16 or C18 fatty acid tail, sophorolipids are slowly being adopted industrially as additives in detergent and other cleaning applications. However, fermentative yields of greater than 100 g/L have stimulated the search for new, novel applications for these molecules. In this presentation we will discuss our efforts in demonstrating

the use of sophorolipids as antimicrobial compounds aimed specifically at the acne-causing bacterium Propionibacterium acnes and show how different biopolymer matrices can be used to enhance the bacteriocidal effects of sophorolipids. We will also show the results of our work in utilizing sophorolipids as additives to various polyhydroxyalkanoate (PHA) biofilms. Scanning electron microscopy revealed that sophorolipids produce a controllable ?dimpling effect? in PHA biofilms which alter the material properties of the films. By varying the amount of sophorolipid that is introduced to the PHA films the number and size of the dimples as well as the porosity created within the film matrix can be controlled which may result in potentially unexplored applications in areas such as tissue scaffolding and bioremediation.

Biological activities of rhamnolipids and their incorporation and release from hydrogel formulations

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The main focus of this presentation is on the incorporation and release of rhamnolipids from several hydrogel formulations that we have been developing. In addition to these observations and results, the following topics will be included: 1. Production of different mixtures of mono- and di-rhamnolipids, 2. Methods for purification of rhamnolipids and separation of their mono- and di-rhamnolipid components, and 3. Biological activities of rhamnolipids on organisms.

Enzymatic synthesis, surface and lipid interaction properties of novel rhamnolipids

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Amongst glycolipidid biosurfactants, rhamnolipids have drawn particular attention as they have several interesting biological properties such as antimicrobial, antiphytoviral, zoosporicidal and plant defense elicitor activities [1-3]. It is generally recognised that these activities must be linked to the interaction of these molecules with constituents of biological membranes [4] but the detailed mechanism is far from being fully understood. The objective of this work is double. First, it aims to investigate a new strategy of synthesis for the production of novel rhamnolipids [5] that could exhibit properties as promising for industrial and environmental applications as their natural counterparts while avoiding the use of the pathogenic Pseudomonas aeruginosa for their production. Secondly, their basic surface properties (critical aggregation concentration, surface tension at CAC and interfacial behaviour of their monolayer) and their interaction with model membranes are investigated in relation with their structure in order to give insight about the mechanism of their biological actions. [1] Vatsa P. et al. Int. J. Mol. Sci. 2010;11:5095. [2] Varnier A-L. et al. Plant, Cell Environ. 2009;32:178. [3] Lang S. et al. Appl. Microbiol. Biotechn. 1999;51:22. [4] Aranda F.J. et al. Langmuir. 2007;23:2700. [5] Nott K. et al. Process Biochemistry, http://dx.doi.org/10.1016/j.procbio.2012.11.019

Drug Delivery Systems based on diacyl arginine surfactants: preparation, characterization and evaluation of their biological activity

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In the last years our group has prepared new diacyl cationic surfactants based on the amino acid arginine, with different structures (gemini, and glycerolipid), characterized by relevant nontoxic and antimicrobial properties as well as rapid biodegradability. In addition, these surfactants from arginine are extraordinarily active in reducing surface tension. Cationic colloidal systems composed by these arginine based surfactants and membrane additive compounds have been characterized by means of size distribution and zeta-potential measurements. Gemini surfactants with the shortest spacer chain formed micelles, while aqueous solutions of pure gemini surfactants with longer spacer made up very big aggregates. The addition of phospholipids or cholesterol changed drastically the aggregation behaviour. The capability of disrupting the erythrocyte?s membrane depends on the hydrophobicity of the molecules and the size of aggregates in the solution. The alkyl spacer chain and the presence of additives also play an important role on the antimicrobial activity. The diacyl-glycerol arginine cationic lipids form stable cationic liposomes by themselves. These formulations can encapsulate different drugs, and the percentage of encapsulated drug depends on the physicochemical properties of the vesicles as well as on the type of drug. The capacity of the systems to vehiculate different molecules was evaluated performing their in vitro drug release profiles. These results suggest that our formulations represent a great innovation in the pharmaceutical field, due to their dual pharmacological function: one related to the nature of the vehiculated drug and one related to the innate antibacterial properties of the surfactant-based carriers.

Soy Protein Fragments as Hydrophilic Components in Surfactants

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The development of protein based surfactant technology has taken many turns over the past one hundred and twenty five years. Early in the history of surfactants, protein based materials emerged as a significant technology that was developed for a number of applications. Over the years, these materials were largely replaced, first with sulfated oils and fatty acids and later with nonionic surfactants based on alkene oxide technology. By the 1950?s, surfactants based on protein technology were largely replaced with materials based on modified fats & oils, petroleum derived intermediates or the combination of the two. Since then, protein based surfactant technology and the related amino acid based surfactant technology has been confined to small volume specialty applications. Working with the United Soy Board, we are carrying out research directed at reestablishing a place in surfactant technology for soy based protein materials. We will report on the progress made in moving this technology from a research program into an early stage development program. Specifically, we will review the properties of newly developed surfactant materials and the prospects for these renewable materials finding commercial opportunities in significant applications and markets.

Eastman GEMTM technology for cosmetic ingredients

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Natural ingredients have always been important in the cosmetics market, while the demand for the use of green processes is becoming more important to both formulators and consumers. While some definitions are still being debated, ?natural? typically refers to the source of the raw materials, and ?green? refers to the processes used to convert starting materials to a finished ingredient. Eastman?s GEMTM technology is centered around a green biocatalytic process to synthesize a variety of cosmetic esters via enzymatic esterifications at mild temperatures. The esterifications are driven to high conversion by removing the coproduct, usually either water from esterification of an acid or a lower alcohol from transesterification of an ester. The mild processing conditions suppress formation of undesirable byproducts that may contribute color or odor. The immobilized enzyme, such as lipase, is easily removed

by filtration. The specificity of the enzymatic conversions and the relatively low reaction temperatures minimize the formation of byproducts, increase yield, and save energy. The GEMTM technology will be exemplified by the manufacture of emollient esters such as 2-ethylhexylpalmitate. The discussion will also include GEMTM processes for the preparation of active ingredients and surfactants.

Surfactants extracted from waste biomass and their use to remove oil from oil-coated sands.

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Previous presentations in this bio-based surfactant session have described the alkaline extraction of wastewater sludge to produce an alkaline solution with surface active properties that rival those of commercial surfactants. We have also described the detergency performance of these extracts and have shown that it approach that of commercial surfactants. This time we present a comparison of the ion composition and performance of alkaline extracts obtained from wastewater sludge (at the University of Toronto) and from compost (at the University of Torino). We will show that the source of biomass produces significant changes in the property of the resulting surfactant, and that the ion composition is also a factor, particularly when it comes to interfacial properties. We will discuss the low and ultralow interfacial tensions that can be obtained with various oils and mixtures of the alkaline extracts and a hydrophobic anionic surfactant, and without added salt. Finally, we will show that the mixture of alkaline waste biomass extracts and a hydrophobic surfactant is capable of improving the removal of oil from oil-coated sands. We will discuss the potential applications of this work in environmental remediation and enhanced oil recovery.

Renewable glucarate-based complexes as auto-dish builders

T. Smith[(1)]
[(1)]Rivertop Renewables, United States of America

The phasing out of phosphate in US automatic dishwashing detergents left a huge performance gap, particularly when it comes to filming and spotting of glassware. While many alternatives to-date do not meet the cost-performance levels of STPP, Rivertop Renewables has developed a high-performing, cost-effective, renewable replacement for phosphate to address the current market challenges. Rivertop has extensively studied a new builder system based on salts of glucaric acid. Glucaric acid is a novel sugar acid readily produced from glucose via Rivertop?s proprietary chemical oxidation technology. The builder system, trademarked Riose?, utilizes an aluminum glucarate complex which has excellent binding strength for calcium and magnesium. Studies have also shown that detergent formulations with Riose have high performance with respect to reduced film and spot formation. Furthermore, the builder?s glucarate component is GRAS and biodegrades naturally. Calcium chelation by the builder is pH-dependent, a property that may well apply to other metals. We refer to this performance characteristic as ?catch and release.? Calcium is caught, or chelated, by the builder in the dishwasher (pH 10+), then released at neutral pH in the wastewater plant. A future area of study will be to determine if ?catch and release? applies to other metals whose migration and concentration could be mitigated to protect freshwater supplies.

Synthesis of succinyl amide gemini surfactant from Adenopus breviflorus seed oil: A prospective corrosion inhibitor of mild steel in acidic medium for the African polpulace

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[(1)]Redeemer's University, Nigeria, Nigeria

Succinyl amide gemini surfactant was synthesised using simple reaction mechanism from the seed oil of Adenopus breviflorus and applied as corrosion inhibitor of mild steel in 0.5 M HCl via weight loss method. The synthesis was monitored and confirmed using FTIR and NMR. The inhibitive mechanism of succinyl amide gemini surfactant was by adsorption which was spontaneous, exothermic and it obeyed Langmuir isotherm with the process being physisorption. The activation energy increased as concentration of succinyl amide gemini surfactant increased with the highest being 135.20 KJ mol-1 at 200 mg/L while the heat of adsorption was -95.25 KJ mol-1 at the same concentration. The result of the corrosion study of mild steel has proved that succinyl amide gemini surfactant is an efficient inhibitor of mild steel corrosion in 0.5 M HCl.

Production of Pure Pinolenic Acid from Pine Nut Oil via Enzymatic Esterification Combined with Urea Complexation

D. No[(1)], T. Zhao[(2)], I. Kim[(3)]
[(1)]Korea University, Korea, Republic of [(2)]Korea University, Korea, Republic of [(3)]Korea University, Korea, Republic of

Pinolenic acid (PLA, C18:3?5) known as a beneficial and unique fatty acid is not available as a pure form. In the present study, pure PLA (>99% purity) was successfully produced from fatty acid from pine nut oil through two-step process including selective esterification using a lipase from Candida rugosa and urea complexation. For the first step, lipase-catalyzed esterification between fatty acid from pine nut oil and lauryl alcohol was carried out at the molar ratio of 1:1 (fatty acid to lauryl alcohol). Three parameters, namely enzyme loading, initial water content in the substrate and temperature were investigated to optimize the reaction condition. Optimum condition of enzyme loading, initial water content, and temperature were 0.1%, 10%, and 5 oC, respectively. At this condition, a maximum PLA content of 43% was obtained from starting material containing 13% PLA. For the second step, urea complexation using PLA-enriched fatty acid from the first step was conducted. As a result, a pure PLA (>99% purity) was obtained at the ratio greater than or equal to 1:4 (fatty acid to urea).

EAT 4/S&D 4.1: Emulsions, Dispersions, and Foams

Chair(s): C. Rojas, AMCOL International Corp., USA; A. Wright, University of Guelph, Canada

Capillary Video Microscopy as a Tool for Developing Double-Emulsion Creams

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Optical/fluorescent microscopy inside narrow capillaries provides micromanipulation of observed microscopic objects to degrees that are not possible without a restriction such as that imposed by the capillary geometry. The reason is a simple one: an observable object that has dimensions comparable to a host-capillary?s diameter are stripped of two degrees of freedom in their movement, while the third degree can be manipulated by flow or the movement of microneedles. The talk will visually summarize a series of phenomena we have observed in our lab, that include coalescence of droplets, swimming of bacteria, multiphase transport in porous media, reaction of overbased lubricants with acid drops. The main topic of the talk will focus on our efforts to make cream-vaccines for immunization through the skin. We are part of a research group that uses several approaches for the achievement of skin vaccination, and our lab?s objective is the making of double emulsions as vehicles of vaccine antigens. Antigens can be simply suspended in the ?internal aqueous phase? of double-emulsion globules, or they may be hosted within liposomes, which in turn are suspended in the double emulsions? ?internal aqueous phase,? thus providing a double-protection system for the

antigen.

The HLB System ? A Time-Saving Guide to Emulsifier Selection

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The HLB (Hydrophile-Lipophile Balance) system provides a means to narrow down the hundreds of emulsifiers available today to a small, manageable list. The system can help save countless hours wasted on the bench by using a ? trial and error? approach. This presentation will: ? define HLB for nonionic surfactants and demonstrate how to calculate HLB values ? explain required HLB for oils to be emulsified and demonstrate a required HLB test ? provide tools for quick implementation of the system back in your lab so you can use the HLB system to optimize both type and concentration of emulsifiers

Nutraceutical Nanoemulsions: Influence of Carrier Lipid Composition and Location on ??carotene Bioaccessibility

?-carotene is used in aqueous-based foods and beverages as a natural color and nutraceutical. We investigated the influence of lipid carrier composition and location on the physical stability, microstructure, and bioaccessibility of nanoemulsions using an in vitro digestion model. ??carotene enriched nanoemulsions (d< 150 nm) were formed using sucrose monoester and lysolecithin as emulsifiers, and corn oil (digestible) and/or lemon oil (indigestible) as oils. The influence of carrier oil composition and location on lipid digestion and ??carotene bioaccessibility was examined by mixing digestible and indigestible oils before homogenization (?oil mixture?), or by preparing digestible and indigestible nanoemulsions separately and then mixing them together (?emulsion mixture?). Lipase induced free fatty acid (FFA) production in the small intestine was more dependent on oil composition than on oil location. The rate and extent of FFA production increased as the amount of corn oil present increased. ??carotene bioaccessibility decreased in the order corn oil (?76%) > oil mixture (?56%) > emulsion mixture (?34%) > lemon oil (?5%), which was attributed to differences in the formation of mixed micelles capable of solubilizing ??carotene. This study provides important information for encapsulating and delivering functional lipids in food and beverage applications.

Physico-chemical Properties, Oxidative Stability and Non-enzymatic Browning Reactions in Marine Phospholipids Emulsions and Their Applications for Food Enrichment

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Marine phospholipids (PL) are more advantageous than fish oil. They seem to have better bioavailability, better resistance and higher content of eicosapentaenoic acids and docosahexaenoic acids than fish oil. The main objective of this study was to explore the possibilities of using marine PL for food enrichment. The secondary objective was to investigate the different aspects of marine PL emulsions including: physico-chemical properties, oxidative stability and non-enzymatic browning reactions while identifying the important factors affecting their stability. The physical and oxidative stability of marine PL emulsions was significantly influenced by the chemical composition of marine PL used. Emulsions with a high oxidative stability could be obtained when using marine PL of high purity with a high content of PL, cholesterol and ?-tocopherol. Non-enzymatic browning reactions (Strecker degradation and

pyrrolization) seemed to influence the oxidative stability of marine PL emulsions. Similar to marine PL emulsions, the oxidative stability and sensory acceptability of marine PL enriched products varied depending on the quality and chemical composition of marine PL used. Overall, this study provided new insights into the oxidative stability of marine PL and preliminary knowledge on the quality of marine PL fortified foods.

Location and Reactivity of Model Ingredients in Emulsions: Effect of Interface Properties and Ingredient Lipophilicity

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[(1)]The Pennsylvania State University, United States of America [(2)]The Pennsylvania State University, United States of America [(3)]The Pennsylvania State University, United States of America

Functional ingredients (e.g., flavors, vitamins, bioactive peptides, drugs) with various properties (e.g., molecular weights, lipophilicities) are often encapsulated in emulsions to enhance their solubility and stability. The performance of oil-in-water (O/W) emulsions as encapsulation systems is controlled to a large extent by the properties of both the emulsion and the ingredient. The objective of this work was to investigate the effect of the interface properties, the ingredient properties and the oil physical state on the location and reactivity of model ingredients in emulsions. Spin probes with various molecular structures and lipophilicities were selected as model compounds and incorporated in nanoscale emulsions, prepared by homogenizing n-tetradecane or n-eicosane into emulsifier aqueous solutions. Emulsifiers with various physical properties were chosen, including proteins and ionic surfactants. The distribution of paramagnetic spin probes between the different phases of emulsions was measured using electron paramagnetic resonance (EPR). The probe molecules partitioned between aqueous, micellar, interfacial and lipid environments, depending on the probe lipophilicity, the fraction of unadsorbed emulsifier and the oil physical state (i.e., liquid or solid). The reactivity of spin probes was measured after addition of water-soluble reactants, and was found to be strongly affected by their location, mobility and by the droplet surface charge. In particular, probe immobilization at the interface resulted in the greatest protection against aqueous reactants.

Structural Impact of Partial Coalescence on ice Cream

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[(1)]University of WIsconsin, United States of America [(2)]University of Wisconsin, United States of America [(3)]University of Wisconsin, United States of America

Partially-coalesced fat globules are important to the structural attributes, texture properties, and stand-up behaviors of ice cream. Commercial vanilla ice cream products with different fat content were analyzed to determine size and amount of partially-coalesced fat globules in the ice cream and their drip-through rates. Partial coalescence was confirmed using light optical microscopy and quantified by laser light scattering . Drip-through rates and height after complete melting were determined by the conventional drip-through test, where the ice cream melts on a mesh screen. Ice cream products containing large partially-coalesced clusters had slower drip-through rates and greater height after melting, whereas those containing smaller globules or clusters collapsed to flow rapidly and completely through the screen. Fat destabilization level, as determined by the relative number of clusters to initial emulsion droplets, did not predict the drip-through or stand-up properties of the ice cream products. A cluster density parameter is being developed to empirically model the relationship between the partially-coalesced fat globules and drip-through rates in ice cream products.

Cancelled - Localization and Stability of ?-tocopherols in Emulsion-based Delivery Systems

Impact of water cut and continuous phase wax crystals on water-in-oil emulsion rheology

D. Rousseau[(1)], S. Ghosh[(2)], S. Haj-shaifiei[(3)]
[(1)]Ryerson University, Canada [(2)]University of Saskatchewan, Canada [(3)]Ryerson University, Canada

The isothermal rheological behaviour of wax-stabilized water-in-oil (W/O) emulsions consisting of light mineral oil, paraffin wax and glycerol monooleate in the oil phase and a dispersed aqueous phase at different water cuts (10-50 wt %) was evaluated. All emulsions were prepared via high-pressure valve homogenization and consisted of the same average water droplet diameter (~30 ?m). Rotational viscometry, oscillatory rheology and creep compliance and recovery were performed on emulsions aged up to 28 days. Freshly-prepared emulsions with a higher water cut had a higher viscosity and storage modulus that those at a lower water cut. With ageing, however, the viscosity and storage modulus of all emulsions increased due to the development of a more pronounced wax crystal network. Supporting results for these findings were acquired with light microscopy, solid wax content, and aqueous droplet size analysis. Overall, this study clearly established that both water cut and continuous phase wax solidification play a significant role in W/O emulsion rheology, with the former conferring a greater influence to emulsion viscosity in the systems studied. Such findings may be used to better understand and tailor emulsion properties in fields of application such as the petrochemical, cosmetics, food and pharmaceutical industries.

Food Grade Water-in-oil Nanoemulsions From a High-pressure Valve Homogenizer and a Microfluidizer

L. Lee[(1)], R. Hancocks[(2)], I. Noble[(3)], I. Norton[(4)]
[(1)]The University of Birmingham, United Kingdom (Great Britain) [(2)]The University of Birmingham, United Kingdom (Great Britain)
[(3)]PepsiCo Intl, United Kingdom (Great Britain) [(4)]The University of Birmingham, United Kingdom (Great Britain)

The purpose of this work was to compare the production of sunflower oil continuous nanoemulsions using a Microfluidizer (high pressure impinging jet) and a high pressure valve homogeniser (HPH). The work investigates the affect of homogenising pressure, pass numbers, viscosity ratio, PGPR concentration and electrolyte addition on the droplet size; and complements previous studies that have explored droplet break-up mechanisms for O/W nanoemulsions [1]. Comparing the energy dissipation in the high pressure devices indicates that the smallest eddies in the system should be of the order of 1 ? 3 ?m. The droplet sizes achieved are from 100 nm after the first pass, reducing to 50 nm after the fifth pass. The continued droplet size reduction and the size of the droplets in comparison to the expected turbulent length scale indicate turbulent viscous flow. Processing at this oil viscosity (0.01 Pa.s) has matched the performance of the HPH and Microfluidizer; this is explained to be a result of minimal coalescence and negligible effects from the impinging jet. The continuous phase viscosity was increased by an order of magnitude, however this did not affect the change in droplet size. Whereas, an increase in the dispersed phase viscosity to the same extent has led to a droplet size increase. This highlights the change in droplet break-up mechanism with flow regime. 1. Lee, L. and I.T. Norton, Comparing droplet breakup for a high-pressure valve homogeniser and a Microfluidizer for the potential production of food-grade nanoemulsions. Journal of Food Engineering, 2012.

Microencapsulated Self-emulsifying Delivery Systems.

E. Acosta[(1)], M. Nouraei[(2)], L. Diosady[(3)]
[(1)]University of Toronto, Department of Chemical Eng. and Appl. Chemistry, Canada [(2)]University of Toronto, Canada [(3)]University of Toronto,

Canada

This presentation describes self-emulsifying and self-microemulsifying delivery systems for food ingredients. The presentation will describe the formulation of the food-grade self-emulsifying systems produced with lecithin-linker systems.

AFTERNOON

ANA 5.1/S&D 5: Emerging Test Methods for Surfactants and Detergents
Chair(s): M. Tsumadori, Kao Corp., Japan; H. Li, Bruker Optics Inc., USA

Characterization of Surfactant Iron Oxide Nanoparticle Interactions Using Isothermal Titration Calorimetry (itc)

Z. Wang[(1)], S. Xu[(2)], E. Acosta[(3)]
[(1)]University of Toronto, Canada [(2)]University of Toronto, Canada [(3)]University of Toronto, Canada

Formation of stable nanoparticle suspensions is important for their potential use in cosmetic, pharmaceutical, environmental, and medical applications. One method to produce stable aqueous nanoparticle suspensions is to adsorb surfactants on the surface of the nanoparticle to create a steric and electrostatic barrier against particle aggregation. However, depending on the structure of the surfactant tail, the charge of the surfactant head group, and the binding of the surfactant to the surface of the particle, one obtains substantially different stabilities. Therefore, a better understanding of surfactant-nanoparticle binding is necessary to design stable suspensions. In this work, the binding between sodium oleate, sodium laurate, sodium dodecyl sulfate, and sodium dodecyl phosphonate and iron oxide nanoparticles was systematically investigated using isothermal titration calorimetry (ITC). Comparing the ITC results and the adsorption isotherm obtained for these systems, in the cases of sodium oleate and dodecyl phosphonate, a strong chemical binding ? beyond a simple physisorption ? takes place in the presence of low surfactant concentrations. However, the formation of higher order structures (e.g. surfactant bilayers) cannot be accurately reflected in the ITC experiments. Those surfactants that exhibited strong chemical binding also produced the more stable suspensions.

Using Inflection Points in Surfactant Blend Properties as a Guide to System Synergies

R. Theiner[(1)], R. Bennett[(2)]
[(1)]Air Products and Chemicals, Inc., United States of America [(2)]Air Products and Chemicals, Inc., United States of America

Neat surfactant behavior is well understood thanks to established models, but blended systems continue to yield synergies that are sometimes unexpected. A process of examining deviation from the anticipated model may be used to simplify the search for such synergies. This paper presents determined critical micelle concentrations for blends of lauryldimethylamine oxide with a common linear alcohol ethoxylate and shows how inflection points outside of linear behavior reveal performance synergies. Although this study is provided as an example, the technique is particularly highlighted.

Quantification of oil extraction from microalgae using conventional solvents and microemulsions

E. Acosta[(1)], J. Chan[(2)], R. Xu[(3)], L. Diosady[(4)]
[(1)]University of Toronto, Department of Chemical Eng. and Appl. Chemistry, Canada [(2)]University of Toronto, Canada [(3)]University of Toronto, Canada [(4)]University of Toronto, Canada

This work describes the process of extraction of lipids from Scenedesmus obliquus microalgae using hexane (a conventional solvent) and three lecithin-linker microemulsions, one continuous in water (Type I), one continuous in the oil phase (Type II) and one bicontinuous in oil and water (Type IV). The fraction of lipids was determined by measuring the lipid content in lyophilized microalgae before and after extraction. To this end, the Folch?s chloroform/methanol extraction method was applied in both cases, and the extracted lipid underwent transesterification followed by GC chromatography to quantify the fatty acid methyl esters (FAMEs) in the sample. We will describe our initial challenges in producing a reliable measurement of the oil content in the microalgae as well as the adjustments we needed to introduce in the Folch extraction methodology. Since the Folch method did not capture the extraction of carotenoids from the microalgae, we adapted a liquid chromatography method to determine the extraction of carotenoids from the samples. We will discuss the relative extraction efficiency for lipids and carotenoids of the solvents explored and the potential advantages and disadvantages of those extraction methods.

Use of acoustic spectrometry to determine drop size distribution of water-in-bitumen emulsions

E. Acosta[(1)], W. Ren[(2)], S. Ng[(3)]
[(1)]University of Toronto, Department of Chemical Eng. and Appl. Chemistry, Canada [(2)]University of Toronto, Canada [(3)]Syncrude Canada Ltd., Canada

One of the biggest issues when trying to characterize emulsions and dispersions is that most of the technologies available require taking a sample of the suspension or emulsion and placing it in a microscope or diluting it for laser scattering techniques. These procedures may affect the morphology of the emulsion or the dispersion. The advantage of acoustic spectroscopy is that it can be used in large concentrated samples, thus minimizing sampling issues. The first half of this presentation will review the principles of acoustic spectroscopy and its use in characterizing emulsions and suspensions. The second half will describe literature examples on the use of this technique as well as our own experience with this technique for analyzing coexisting emulsions and microemulsions, samples of bitumen emulsions and other turbid emulsions. We will describe the potentially powerful use of the technique to access information that is not available from other techniques, but the importance of running controls and complementary techniques to chose the right model to analyze the sound absorption spectra, which is the primary set of data obtained from the instrument.

Surfactants and Detergents Poster Session

Chair(s): M. Wint, Amway Corp., USA

Determination of Phytotoxic Effects of Some Cationic Surfactants on Epicuticular Structure of L. minor L. Observing by SEM

G. YILMAZ[(1)]
[(1)]TRAKYA UNIVERSITY, Turkey

Surfactants are widely used in household cleaning detergents, personal care products, textiles, paints, polymers, pesticide formulations, pharmaceuticals, mining, oil recovery and pulp and paper industries. This study describes the toxic effects of cationic compounds on a common and widespread aquatic vascular plant, Lemna minor. Surfactants

bind to proteins as well as to phospholipids influencing (stimulating or inhibiting) enzyme activity and membrane permeability. The mechanism of phytotoxicity of surfactants is poorly understood on penetrating plant tissues. Because of that in this study, cationic surfactants Cetyltrimethylammonium bromide (CTAB) and Gemini surfactant (16-2-16) were used. The phytotoxic effects of CTAB and Gemini surfactants were determined on aquatic plant Lemna minor after treated with 20% concentration for 48 hours at 16 ± 0.5ºC. 5 ml. added to the 25 ml tap water in each Petri dishes in laboratory conditions. After 48 hours, toxic effects of (CTAB) and Gemini surfactants were determined by scanning electron microscope on the epicuticular structure of leaves belonging Lemna minor L. It was determined that cationic surfactants made cuticular shrinks on cuticula as given in SEM micrographs.

Monoglyceride Oily Soil Detergency : Effect of Added Salt

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[(1)]The Petroleum and Petrochemical College Chulalornkorn University, Thailand [(2)]Chulalongkorn University, Thailand

The objective of the research is to apply a microemulsion-based formation for remove of monoglyceride oily soil from fabric at low salinity. Give the chemical formula of surfactant, extended surfactant was used to form microemulsions with monoglyceride oil at temperature slightly about its melting point (28-38 C). In order to obtain a better understanding, the dynamic interfacial tensions (IFT) of all studied micro emulsion were carried out. For detergency testing, methyl palmitate or palmitic acid methyl ester stained polyester/cotton blend (65:35) fabric was cleaned using a Terg-O-Tometer at different total surfactant concentrations and washing temperatures. In addition, the re-deposition of removed oily soil was also investigated. From the preliminary results showed that the polyester fabric had higher removal efficiency than the cotton fabric. In addition, the re-deposition of the monoglyceride oil onto the fabric was less than 1%.

Formulation Design for Targeting Delivery of Surfactant-coated Iron Oxide Nanoparticles to tce Zone

Z. Wang[(1)], E. Acosta[(2)]

[(1)]University of Toronto, Canada [(2)]University of Toronto, Canada

In situ degradation of dense non-aqueous of liquid phase (DNAPL) can be achieved by injecting zero-valent iron nanoparticles (NZVI) to the contaminant zone. This technique is challenging due to the poor stability and mobility of NZVI in porous media. Therefore, formation of stable NZVI dispersions and targeting delivery nanoparticles to TCE zone can be crucial for this technique. This presentation discusses several strategies to deliver iron-based nanoparticles to the dense non-aqueous phase liquid (DNAPL) zone. Iron oxide nanoparticles were selected in this work as surrogates for NZVI as they have similar chemical composition on their surface. Sodium oleate (SO) forms pre-adsorption bilayer on the iron oxide nanoparticles with the objective of obtaining highly stable suspensions. The hydrophilic-lipophilic nature of SO-coated iron oxide nanoparticles are adjusted using various strategies: via the increase in CaCl2 concentration, the decrease of pH, and via the addition of benzethonium chloride (BC). The formulation modified by the mixture of SO and BC shows promising application in targeting delivery due to the high stability in aqueous phase and the preferential partition effect to trichloroethylene (TCE). Moreover, this formulation shows the affinity on TCE contaminated sands based on column test results.

Fatty Acid Diethanolamide Replacement by a High Active Betaine

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[(1)]Evonik Industries, United States of America [(2)]Evonik Industries, United States of America

Fatty acid diethanolamides like cocoamide DEA have a secondary amine residue which can cause nitrosamine contamination in the final product. It is especially problematic when these nonionic surfactants are used in manual cleaning applications like hand soaps and manual dish wash detergents. To overcome this deficiency, a high active cocamidopropyl betaine was used as a replacement. Comparable or better foam profile was verified via foam tests at various temperatures, water hardness, and soil levels. Using this new, high active betaine an additional benefit can be provided: skin moisturizing. The chemistry and benefits will be discussed in the presentation.

Spectroscopic Study of the Interaction Between C.i. Reactive Red180 With Cationic Gemini Surfactant in

Aqueous Solution

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[(1)]Trakya University, Turkey [(2)]Trakya Universitesi, Turkey [(3)]Trakya University, Turkey

In the present study, the gemini surfactants of type alkanediyl-?-?-bis (alkyldimethyl ammonium) dibromide with different alkyl groups referred as ?m-2-m? (m= 10, 12 and 16) and with different spacer groups referred as ?16-s-16? (s= 2, 6, 10 and Ar (8)) have been synthesized, purified and characterized in our laboratory. The influence of these surfactant and the monomeric cationic surfactants (DTAB and CTAB) on spectral properties of an azo dye in aqueous solutions has been investigated by means of UV-vis spectroscopy in submicellar and micellar concentration range. The spectral signature of the polarity of the azo dye C.I. Reactive Red180 (RR180) exhibits sensitivity to the polarity of the dyes environmental. The aggregation of surfactants and dye takes place at surfactant concentration far below the critic micelle concentration (CMC) of the individual surfactant. The CMCs of the gemini surfactant-dye solutions are found to be much lower than those of the corresponding monomeric surfactant-dye solutions. The short-range hydrophobic interactions are very important factors as the long-range electrostatic forces on the dye-surfactant aggregation. It was found that the effect of the hydrophobic alkyl chain length is more important than that of the spacer.

Phytotoxic Effects of Three Surfactants: Dbsna, sds and Gemini Surfactant (16-2-16) on Allium Cepa l. Plantlets

F. Dane[(1)], S. Leventer[(2)], H. Akbas[(3)], F. Öztürk[(4)], G. Yilmaz[(5)]

[(1)]Trakya University, Turkey [(2)]Trakya University, Turkey [(3)]Trakya University, Turkey [(4)]Trakya University, Turkey [(5)]Trakya University, Turkey

In this study, two anionic surfactant, Sodium dodecyl benzene sulfonate (DBSNa) and Sodium dodecyl sulfonate (SDS), and one dimeric cationic surfactant, Gemini surfactant (16-2-16) were evaluated under laboratory conditions using onion (Allium cepa L.) as a test material. Dimeric cationic surfactant, gemini surfactant (16-2-16), was synthesized in our laboratory. All solutions were prepared with tap water. The phytotoxic effect on root were determined after 120 hours of treatment. In previous studies, Surfactants used in this study were found to be very toxic at 0.5%, 0.2%, and 0.1% (w/v) concentrations. Consequently, the effects of surfactants have a marked impact on human health care, biotechnology, environmental protection and agrochemistry. It is important that the determined EC50. In addition, it must be selected an appropriate surfactant which has minimal toxicity and maximal benefits for each purpose. So in this study, diluted concentrations of surfactants used at three different concentrations (stock solution contains 5 g.sur./1000ml water) (1/8) and diluted solutions of (1/16) and (1/32)) were used.]. The phytotoxic effects were observed on onions which treated by anionic surfactants. Stimulatory effects only occurred on onions treated by Gemini (16-2-16) (cationic)at 1/32 concentrations while inhibitory effects were observed on onions treated by all concentrations of SDS and DBSNA. It was observed that inhibitory effects increased with increasing concentrations of SDS and DBSNA.They were very toxic while Gemini (16-2-16) was less toxic.

Next Generation Hybrid Polymers - a More Sustainable Solution

M. Vanderhoof[(1)]

[(1)]AkzoNobel Surface Chemistry, LLC, United States of America K. Rodrigues[(1)]

[(1)]AkzoNobel Surface Chemistry, LLC, United States of America

AkzoNobel has developed a new, biodegradable biopolymer technology for the Fabric and Cleaning marketplace. Based upon the combination of selected polysaccharides and synthetic monomers, the Hybrid Polymers of this technology biodegrade in the environment, offer a preferable carbon footprint, and are effective in replacing synthetic polymers in formulations such as automatic dishwash and laundry detergents. This 2nd Generation technology provides a sustainable and cost effective alternative to existing synthetic options. This poster will provide insight on the latest developments with AkzoNobel Surface Chemistry?s readily biodegradable Hybrid Polymer Technology. Specifically, the performance of these polymers in automatic dishwash and laundry detergents, and their positive environmental aspects will be reviewed, including lifecycle analysis.

Particle Based Rheology - Adjus for Structured and Isotropic Liquids

(1)

S. Mohammed
(1)Evonik Degussa Corporation, United States of America
Overview of the core physical and chemical properties that affect particle based rheology. With focus on the various visco-elastic profiles that can be factored into formulation design. Specific application areas for these concepts include structured and isotropic liquids, suspension medium, concentrated liquids, gels, and pastes. Product forms can include detergents, cleaners, and toothpaste.

Designing Controlled Release Systems Based on Silicon Dioxide

S. Mohammed(1)
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By utilizing various particle morphologies, systems that absorb and contain large quantities of liquid actives can be designed. Both absorption and agglomeration mechanisms are possible; yielding encapsulates that off a wide range of release triggers. Triggers based on mechanical attrition, displacement effects, and chemical change, are possible. This technology is directly applicable to formulation designs in the areas of controlled or delayed released, active protection, and compatibility enhancement.

Optimization of Builders in Automatic Dishwashing Detergent

C. Caires(1), E. Satchell(2), R. Miller(3)
(1)BASF, United States of America (2)BASF, United States of America (3)BASF, United States of America
We have conducted a mixture design to determine the optimal builder concentration for automatic dishwashing detergents. We looked at mixtures containing combinations of soda ash, sodium silicate, sodium citrate, methylglycinediacetic acid (sodium salt), and acrylate co-polymers. We used both visual methods and a digital imaging analysis tool (DIAT) to evaluate the spotting and filming performance.

Aminosiloxanes in Laundry Applications

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Fabric softener formulations made with biodegradable active materials have been commercially available for over 20 years. The previous generations of softener actives have been in decline due to their negative environmental impact, but they have performance characteristics that are superior to current ester quat based actives, particularly ester quats derived from triethanolamine (TEA). Softener actives are typically greater than 80% dialkyl quat by weight. TEA ester quats, on the other hand, are mixtures of mono-, di-, and tri-ester quats. Only the di-ester quat, which is about 50% of the composition by weight on a normalized basis, contributes to the softening of fabrics. Due to this inherent compositional difference, TEA ester quats must be dosed in larger quantities or employ boosters to achieve equal softening performance compared to alkyl quats. In general, siloxane additives boost overall performance and impart additional benefits, such as reduced wrinkling and improved ironing characteristics. Specifically, a new aminosiloxane has been developed that significantly improves the fabric softening and rewet performance of TEA ester quat formulations. Formulation procedures and comparative results will be discussed.

"SYNTHESIS AND STUDY BIOLOGICAL ACTIVITY OF SOME SCHIFF BASE NANOPARTICLES AND THEIR APPLICATIONS IN EGYPTIAN PETROLEUM FIELDS"

N. AbdelRahman(1)
(1)Pharma Swede Egypt, Egypt
Summary and Conclusions i SUMMARY AND CONCLUSIONS In this thesis, we prepared four monoSchiff bases and one dischiff base cationic surfactants. 1- The monoquaternary Schiff base surfactants were prepared by reacting m-aminopyridine and different fatty esters of ketoglutaric acid to produce the dialkyl monoSchiff bases. Then the Schiff

bases were quaternized by ethyl iodide (4-compounds). 2- The diquaternary dischiff base cationic surfactant was prepared by coupling of m-aminopyridine and acetyl acetone in (2:1) molar ratio then the obtained dischiff base was quaternized by excess of ethyl iodide (1-compound). 3- The diquaternary surfactant was loaded on silver nano particle to obtain the nano-sized diquaternary surfactant by the reduction method to prepare the silver nanoparticles. (1-compound) 4- The prepared cationic surfactants were complexed with transition metals; namely (Cu, Co, Ni, and Mn) to obtain the different metal complexes. (20-Compounds). 5- All the chemical structures of 25- compounds (not nano sized diquaternary) were investigated by using:- A- Elemental analysis:- which showed the high purity of the prepared compounds. B- Infrared spectroscopy: - which showed the identical function groups in the chemical structure as represented in the different schemes. C- Proton nuclear magnetic resonance (^{1} HNMR):-which showed the distribution of the protons in the chemical structure as expected. 6- The surface activity of the prepared compounds determined by using Summary and Conclusions ii surface tension, Interfacial tension measurements, Emulsification power and Partition coefficient values. the surface activity measurements showed the good activity of the data of critical micelle concentration .effectiveness, efficiency, maximum surface excess and minimum surface area the surface activity of the compounds were confirmed by the thermodynamic data, e.g., standard fee energy changes of adsorption and micellization. 7- The prepared cationic monoquaternary surfactants were applied as corrosion inhibitors

Lysine based cationic surfactants at the air-water interface. Mixed monolayers with DPPC: An investigation into the antimicrobial activity

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Antimicrobial resistance to antibiotics is a major global public health threat, thus development of new antimicrobial compounds is of great significance in biomedicine chemistry. Cationic surfactants exhibit antimicrobial activity and have been used as disinfectants in hospitals and in food and pharmaceutical industry. These types of applications require compounds that do not present hemolytic or cytotoxic activities. To search for new antimicrobial agents, our group has synthesized cationic surfactants from different amino acids. Amino acid based surfactants can be prepared from renewable raw materials and are characterized by their high biodegradability and moderate toxic levels. We report studies that contribute to elucidate the relationship between surface activity of three lysine based surfactants and their antimicrobial activity. To this end, the adsorption properties at the air/liquid interface of spread monolayers were studied. Under saline conditions their spread monolayers can be compressed. Mixed monolayers with DPPC showed an expansion of the DPPC monolayer which suggests interactions of the compounds with DPPC molecules that strongly depend on the surfactant structure and on the position of the cationic charge. The antibacterial activity against Staphylococcus aureus and Escherichia coli bacteria has been performed by electron microscopy observation. The three surfactants caused multiple forms of damage as evidenced by structural alterations, leakage of internal material and cell destruction on the bacteria.

RHAMNOLIPID CHARACTERIZATION AND ITS INFLUENCE ON DPPC BILAYER ORGANIZATION.

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The pressing need for more biosustainable, biocompatible and biodegradable surfactant based products make the study of biosurfactants an important area of research. Biosurfactants are surface active biomolecules that are produced by a variety of different microorganism. Rhamnolipids produced by Pseudomona aeruginosa consist of one or two rhamnose molecules linked to one or two molecules of hydroxydecanoic acid. Rhamnolipids have the two main properties of surfactants, show strong surface activity and self assembly in water. Understanding their fundamental physico chemical properties and how these relate to their biological roles are key to their wider exploitation. Despite the importance that the interaction between rhamnolipids and membranes might play in their biological mechanism of action very little is known, especially regarding rhamnolipid-phospolipid molecular interactions. The aim of this work was to study the ability of RL8 mixture to form vesicles in absence and presence of the phospholipid DPPC. We employed size and Z- potential to characterise the size and the external charge of the vesicles and SAXS to measure the vesicle bilayers characteristics. The biosurfactant forms ordered bilayers with long repeating distances, these long

repeating distances are stabilized by the charging of the bilayer and also by a strong fluidity of the bilayers. The ability of RH to increase the fluidity of DPPC bilayers may be related with the strong hemolytic power of these molecules.

The Science and Formulation Aspects of ADW Rinse Aids

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Rinse aids are widely used in Automatic Dishwashing (ADW) to reduce spotting due to droplet formation, improve drying performance by facilitating drainage, and enhance the perceived overall cleaning of wares. This talk will focus on the ingredients of consumer rinse aid formulations that enable performance and product stability. First, performance will be discussed in the context of the primary performance ingredients ? the surfactants. The general ?rules? for choosing rinse aid surfactants will be examined relative to the fundamental metrics of wetting and defoaming. Second, formulation stability will be discussed in terms of the compatibility index, or the overall cloud point of the formulation. The effects of traditional hydrotropes will be presented as well as approaches to choosing nontraditional hydrotropes. Finally, formulation prototypes will be shown where applicable with accompanying performance attributes.

Jatropha and Pongamia oil derived sophorolipids: Characterization and application in laundry detergents

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Sophorolipids (SLs) are glycolipidic biosurfactants suitable for variety of biological and physicochemical applications. In order to compete with the synthetic surfactants, production cost of SLs should be lowered. For the same purpose, here the attempt has been made to reduce the raw material cost by using non-edible oils namely Jatropha and Pongamia. Through optimization of parameters and resting cell method, the yields 15.25g/l and 19.3g/l could be achieved for Jatropha oil derived SL (SLJO) and Pongamia oil derived sophorolipid (SLPO) respectively with 1% v/v oil feeding. Both displayed good surfactant property with the Critical Micelle Concnetration (CMC) values 9.5mg/l for SLJO and 62.5mg/l for SLPO. Keeping the prospective use of these SLs in mind, the physicochemical properties were checked along with emulsion stability under temperature, pH stress and in hard water. Also antibacterial action and stain removal capabilities in comparison with commercial detergent were demonstrated. SLs enhanced the detergent performance. Based on the results, it can be said that SLs have utility as fabric cleaner with advantageous properties such as skin friendly nature, antibacterial action and biodegradability. So SLs are potential green molecules to replace synthetic surfactants in detergents so as to reduce harm caused to environment through detergent usage.

Emulsification Properties of Surfactin, and Other Food-based Biosurfactants

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Surfactants are amphipathic molecules that consist of both hydrophilic and hydrophobic moieties, and are able to lower surface tension of liquids and thereby mixing immiscible liquids together. The synthetic surfactants are produced through organosolvent processes based on high temperature esterification reactions. However, food-based or microbially or produced surfactants are naturally occurring and reduce the need for harsh reaction conditions. Surfactin, a biosurfactant produced with Bacillus subtilis fermentation was compared with other food ingredients that show surfactant properties?SDS, lecithin, soy protein isolate, bovine serum albumin, and SSL. Emulsification activity and emulsification stability were compared by preparing oil-in-water emulsions. Effect of pH (3 and 7) and ionic strength (0, 0.5, 0.75, 1.25, and 1.75) on emulsion properties was also compared. Size distribution with time was also monitored to compare both the initial particle size and the degree of coalescence. Surfactin had comparable emulsifying stability (rate of change in absorbance, 0.0086 min-1) as SPI (0.0088 min-1) and was more stable than lecithin, soy protein isolate, bovine serum albumin, and SSL. Surfactin was twice as much stable in higher ionic conditions than other surfactants studied, indicating its usefulness in food and industrial applications.

Synthesis and Properties of Novel Chemocleavable Surfactants Bearing a Sucrose Derived from Diethyl

Tartrate

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Surfactants are used in many applications, such as detergents, paints, toiletries and pharmaceuticals. The development of surfactants with excellent surface-active properties, additional functions, or good biodegradability has become desired. Therefore, it has come to be great interest to develop "chemocleavable" surfactants which are designed to decompose into non-surface active species under mild conditions after fulfilling their original functions such as emulsification, solubilization, and micellar catalytic activity. One-chain and double-chain chemocleavable nonionic surfactants bearing a 1,3-dioxolane ring were prepared from diethyl tartrate without any expensive reagents or special equipment. A sucrose was used as hydrophilic group. We clarified that they have good surface-active properties, and the decomposition function in acid water. Biodegradability of the surfactants was evaluated by an oxygen consumption method according to the guidelines which was based upon the OECD 301C with activated sludge. The biodegradabilities of these chemocleavable surfactants after 28 days are more than 60 %. They have acid-decomposition property and good biodegradability.

Synthesis and Evaluation of surface active properties of ester based cationic imidazolium monomeric surfactants.

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New imidazolium cationic surfactants have been synthesized by esterification of halogenated carboxylic acids with long chain fatty alcohols furnishing respective esters (dodecyl-2-chloroacetate, tetradecyl-2-chloroacetate, hexadecyl-2-chloroacetate, dodecyl-2-bromoacetate, tetradecyl-2-bromoacetate and hexadecyl-2-bromoacetate) followed by their subsequent treatment with 1-trifluoro acetyl imidazole resulting into the formation of title monomeric surfactants: 3-(2-(hexadecyloxy)-2-oxoethyl)-1-(2,2,2-trifluoroacetyl)-1H-imidazol-3-ium chloride (7); 3-(2-(tetradecyloxy)-2-oxoethyl)-1-(2,2,2-trifluoroacetyl)-1H-imidazol-3-ium chloride (8); 3-(2-(dodecyloxy)-2-oxoethyl)-1-(2,2,2-trifluoroacetyl)-1H-imidazol-3-ium chloride (9); 3-(2-(hexadecyloxy)-2-oxoethyl)-1-(2,2,2-trifluoroacetyl)-1H-imidazol-3-ium bromide (10); 3-(2-(tetradecyloxy)-2-oxoethyl)-1-(2,2,2-trifluoroacetyl)-1H-imidazol-3-ium bromide (11) and 3-(2-(dodecyloxy)-2-oxoethyl)-1-(2,2,2-trifluoroacetyl)-1H-imidazol-3-ium bromide (12). Their identifications are based on IR, 1H, 13C NMR, DEPT and Mass spectral studies. The dynamics of surface activity of these surfactants have also been investigated in the presence of sodium halides (NaCl and NaBr) by surface tension measurement. A series of useful parameters like critical micelle concentration (cmc), surface tension at the cmc (?cmc), adsorption efficiency (pC20), effectiveness of surface tension reduction (?cmc), Gibbs free energy of the micellization (?G0mic) and Gibbs free energy of adsorption (?G0ads) have been determined from the measurements obtained by surface tension and conductivity method. Further with the application of the Gibbs adsorption isotherm, maximum surface excess concentration (?max) and minimum surface area/molecule (Amin) at the air-water interface were also estimated. Thermal stability of these long chain cationics have been measured by thermal gravimetric analysis under nitrogen atmosphere. Analysis of thermal stability measurement indicated that the thermal stability of these long chain imidazoliums increase with an increase in chain length.

Improving the Performance and Reducing the Cost of Laundry Formulations with 100% Sustainable Poly(Sodium Itaconate)

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Poly(sodium itaconate) is a cost effective and 100% sustainable alternative solution to phosphates, citric acid, and petroleum-based chelants such as EDTA and other aminoacetates. This water-soluble polymer is produced from itaconic acid, a monomer obtained by fermentation of carbohydrates with Aspergillus terreus. All of the carbon in poly(sodium itaconate) are from renewable resources, and the polymer is readily biodegradable. The polymer has exceptional calcium binding capacity, which was proven to boost primary detergency properties in laundry formulations. The anti-encrustation and soil anti-redeposition properties of this polymer have also been quantified effectively. In addition poly(sodium itaconate) showed good enzymatic stability, demonstrating it has efficacy in both

powder and liquid laundry formulations. Incorporating only 1 gram of the polymer per washing dose into existing leading national brand powder laundry formulations lowered the overall cost of the detergent with no loss of soil removal performance.

Program