2009 Annual Meeting Abstracts

Surfactants and Detergents

MONDAY

MORNING

S&D 1: Green Theme: LCA, SUSY, Green C/N

Chair(s): M. Ventura, Church & Dwight Co. Inc., USA; and G. van Buskirk, Clorox Services Co., USA

Biodegradable Chelating Agent Derived from Renewable Feedstock: Economic Replacement of EDTA and NTA. J. LePage, B. Parry, AkzoNobel Functional Chemicals LLC, Chicago, IL USA

L-glutamic acid (MSG) can be produced by fermentation of sugars from various renewable sources. MSG can be readily modified via addition of two carboxymethyl groups on the primary amine. The result is a fairly strong readily biodegradable chelate: L-glutamic acid, N,N-diacetic acid or GL for short. GL exhibits a highly favorable toxicological profile. From a performance standpoint GL's metal chelating ability mimics and is a possible replacement of NTA and EDTA. However GL may offer even greater formulation flexibility due to its very high solubility from low to high pH. This property should allow formulators to reduce the water content of cleaning products for example and thus further reduce packaging and transport impact of consumer goods.ASTM-D6866 testing shows GL is ~ 53 % biobased. With positive environmental and health profiles and possessing favorable chelating and physical properties, GL promises to be a renewable based alternative for conventional chelates / phosphates in diverse application areas.

Green Home Care Formulary. Markus Doerr, Stephen Gross, Anna Kvecher, Cognis Corporation, Ambler, PA, USA

Increasing pressure from the public makes it necessary to produce household chemicals which are mainly based on plants with less hazardous ingredients. In this respect a "Green" or "Natural" Formulary for All Purpose, Bathroom, and Glass cleaners plus Laundry Liquids, Manual Dish detergents and Cleaning Wipes was developed with the target to reduce or eliminate questionable or undesirable products like derivatives of nonyl phenol and ethylenoxide, petrochemicals, solvents, etc.Since there are numerous eco-labels available and a unique definition of "Green" and/or "Natural" does not exist, a simple and easy system was created in order to classify products and formulations. All formulations were categorized against these definitions, and their performance was tested vs. market benchmarks. In nearly all cases, it can be shown, that low cost and a high degree of "Green"/"Natural" are not prohibitive for an excellent performance.

Sustainable High Performance Enzyme Solutions for Automatic Dishwashing. N.E. Prieto, V.M. Casella, T.J. Neal, Novozymes NA, Inc., USA

Companies are rethinking tomorrowâ??s detergents striving to meet stricter environmental regulations and respond to the increasing demand for environmentally friendly products, while still meeting the performance expectations of the consumer. In doing so formulators are most interested in sustainable materials that do not compromise performance. Enzymes solutions help meet these demands replacing traditional detergent ingredients while maintaining a high performance and environmentally friendly detergent profile. A study was conducted to evaluate these benefits in automatic dishwash detergent application. Results indicate wash performance can be maintained in non-phosphate containing automatic dishwash detergent products when including enzymes. A considerable environmental improvement can also be achieved when enzymes displace some of the conventional detergent raw materials like phosphate.

CANCELED - Innovative Approach to Reduce Environmental Impacts on Home Laundry. Takanori Kotera, Kao Corporation, Household Products Research Laboratories, Wakayama, Japan

In order to make the sustainable society possible, it is essential for us to suppress the environmental impacts. One of the methods to quantify the size of these impacts from our products is to count the CO_2 emission volume. We

evaluated the environmental loads of raw materials, manufacturing processes, transportation, bio-degradation of sewage water, packaging, electricity, tap water and waste water treatment used for washing regarding the laundry detergent by using the LCA (Life Cycle Assessment) methodology. Based on this evaluation above, the relatively major part of environmental impacts in our washing process is clarified and the new technology to suppress these burdens will be discussed in this presentation. The trend of the change in laundry detergents and washing machines are shown and related CO_2 emission volumes are compared with that of total household origin. Based on the result of this comparison, the more important factor rather than the simple product-related factor will also be discussed.

Viscosity Studies of Shampoos Based on Surfactants Derived from Natural Renewable Resources. Vijayanand Magar, Bhushan Sonchal, Shrinivas Kothekar, Shamim Momin, Dept. of Oil Technology, Institute of Chemical Technology, N.P. Marg, Matunga (E), Mumbai-400 019, India

Surfactants derived from natural renewable resources are of great interest for research because of growing concern about the eco-friendly products. Environmental concerns have provided the driving force to replace petrochemical-based surfactants with those based on naturally occurring renewable sources like vegetable oils, carbohydrates, etc. The present work deals with the viscosity study of shampoos using Alkylpolyglycosides (APG). Functionally and chemically, APG are nonionic surfactants consisting of hydrophilic sugar group and hydrophobic fatty alcohol group. APG are biodegradable surfactants derived from natural renewable resources. National Toxicology Program found that diethanolamine is readily absorbed through the skin and accumulates in organs, such as the brain, where it induces chronic toxic effects. Coco-diethanolamine (CDEA), a prominent member of amine family acts as viscosity modifier and foam booster in shampoo formulations. Hence, in our study we have tried to replace amine based surfactant with APG which are found to be effective viscosity modifiers and foam boosters. The viscosity of the formulated shampoos is comparable with the commercial and amine based shampoos. APG-based shampoos give stable abundant foams and better viscosity indicating that APG are good viscosity modifiers and eco-friendly surfactants for shampoos.

CANCELED - Development and Properties of a New Eco-Friendly Cationic Hair-Conditioning Agent. T. Sakai[1], K. Inoue[1], M. Minguet[2], P. Castán[2], N. Nishiyama[3], M. Yamane[3], [1]Kao Corporation, Material Science Research Laboratories, Wakayama-shi, Wakayama, Japan, [2]Kao Chemicals Europe, Barberà del Vallès, Barcelona, Spain, [3]Kao Corporation, Safety Science Research Laboratories, Ichikai-machi, Haga-gun, Tochigi, Japan

Cationic surfactant is an important material used in hair conditioner, fabric softener and other industrial products. By investigating the relationship between the aquatic toxicity and the chemical structures of two types of mono-alkyl cationic surfactants, alkyl trimethylammonium salts and alkyl dimethylamine salts, we have developed *N*-[3-(dimethylamino)propyl]docosanamide salt (APA-22). In evaluation of aerobic and anaerobic biodegradability, APA-22 was shown to exhibit "rapid biodegradability". Additionally, the toxicity values of APA-22 to algae, daphnia, and fish were all greater than 1 mg/L, indicating that the environmental toxicity of APA-22 is less than other existing monoalkyl cationic surfactants. The hair-conditioning properties APA-22 exhibits are better than the ordinary hair-conditioning agents used in the world. On the other hand, APA-22 has excellent solubility in water with a solubility limit over 10-times larger than that of other APA type surfactants with shorter alkyl chain lengths at 25°C. This excellent solubility of APA-22 in water is considered to be a result of the unique stepwise aggregation behavior under the temperature condition below Krafft point.

Green Surfactant Solutions based on Derivatized Alkyl Polyglucosides. R.J. Coots, Colonial Chemical, Inc., South Pittsburg, TN, USA

This presentation introduces a unique series of anionic, cationic, and amphoteric surfactants based on derivatized alkyl polyglucoside building blocks. These patented surfactants are based on naturally-derived, sustainable, non-petroleum raw material feed stocks. These new surfactants are shown to be very mild, yet very effective surfactants. The mildness of these products is measured by both skin irritation and eye irritation testing and compares very favorably to traditional surfactants.Part of this presentation is also dedicated to a discussion of the definition of a 'Green Surfactant'. While there are many terms and definitions in the marketplace now, there are some practical ways to define 'Green' in the context of surfactants specifically, as well as personal care ingredients in general. This talk will describe the monomer version of these derivatized APG surfactants as well as a polymeric version of alkyl polyglucosides which is

then derivatized to introduce useful functionality. These surfactants are suitable for applications in industrial cleaning and personal care, and they offer formulators new technology for making greener products.

S&D 1.2: General Surfactants I
Chair(s): C. Choy, CKC Consultants, USA; and J. Billman, Genencor, USA

Rapid Emulsifier Selection and Evaluation of Emulsion Stability for Reformulation. Titus Sobisch[1], Dean Dinair[2], Dietmar Lerche[1], [1]LUM GmbH, Berlin, Germany, [2]LUM Corp., Volente, TX, USA

Selection of emulsifiers and evaluation of emulsion stability is a frequent task. This relates to practical issues like formulation of emulsions, optimization of preparation conditions, quality control, shelf life estimation and breaking of emulsions. Due to European legislation (REACH) many companies are facing the problem to replace proven components in their formulations. This also applies to emulsifiers and emulsion based products.A multisample technique based on analytical centrifugation is presented which allows for an accelerated study of creaming, sedimentation and of separation of oil and water phases. Not only information on the extent of phase separation is provided but also the kinetics are measured in-situ.The method was applied to check for alternatives to nonyl phenol based surfactants as emulsifiers for silicone oil-in-water emulsions. Due to the multisample approach one centrifugal run with 12 different samples was sufficient to identify more environmentally benign emulsifiers with identical or better performance.The primary destabilization mechanism for all emulsions was creaming, however, most emulsions showed phase inversion when a critical phase ratio was reached inside the cream layer. By increasing the polarity of the alternative emulsifiers the risk of phase inversion could be rigorously reduced.

Study in Eco-Friendly Detergent Formulation for Removing Heavy Greasy Soil. Jitendra Tongaonkar, Shamim Momin, Institute of Chemical Technology, N.P.Marg, Matunga (E), Mumbai 19, Maharashtra, India

Surfactants are amphiphilic molecules that consist of hydrophilic and hydrophobic structures. Surfactants play an important ingredient in all the detergent formulations. As it is a base component, the performance of the detergent is mainly due to the high influence of surfactant properties and their characteristics in the aqueous solution. The principal properties of surfactants are adsorption, surface tension, interfacial tension, micelles, wetting, foaming and emulsification performance. These properties play an important factor in heavy greasy soil removal from the textile fabrics by using appropriate detergent formulation. The aim of the present study is to formulate phosphate free detergents with the use of Alfa Olefin Sulfonate, Linear Alkyl Benzene Sulfonate, Sodium Lauryl Sulphate and Alkyl Polyglycosides as such in combination with other non-ionic surfactants. Initially, these surfactants are analysized for physicochemical properties. These phosphate free detergents with Alkyl Polyglycosides formulations are found to be Eco-friendly. The formulated detergents were evaluated for removing heavy greasy soil from the various fabrics such as Cotton, Polyester and Polyester/Cotton mix. The performances of detergency are measured under different condition of washing such as temperature and water hardness.

Rapid Formulation Development for Lower VOC Detergents and Cleaners. M. Busby, A. Argenton, Dow Chemical, USA

There is a drive to modify cleaner formulations due to pressure from environmental regulations, labeling laws, and greater awareness of environmental issues by consumers. Specifically, the proposed new rule for VOC content mandates a maximum of 0.5% and proposes an effective date of January 1, 2011.To address this issue, various VOC exempt solvents have been incorporated into a number of typical cleaning formulations. These formulations have been tested for stability and efficacy. The results from this work can be used as a starting point for reformulation of a wide range of cleaners to meet the new VOC rules when they take effect.Computer modeling for formulation development and rapid formulation tools to prepare samples and screen physical properties and cleaning performance can then be used to quickly optimize products.

Lyotropic Liquid Crystals Formed in Surfactant/Ionic Liquid/Water Systems. Zhongni Wang[1], Zhengwu Wang[2], [1]College of Chemistry, Chemical Engineering and Materials Science, Shandong Normal University, Jinan, Shandong,

China, College of Agriculture & Biology, Shanghai Jiaotong University, Shanghai, China

The cohesive energy increases with the increase in the hydrophobic chain of surfactant and the rich phase behavior would be expected in a long chain surfactant system. Several liquid crystals, including lamellar phase, hexagonal phase and micellar cubic phase have been found in aqueous solutions of oleyl polyoxyethylene ether surfactant when adding ionic liquid either bmim-BF_4 or bmim-PF_6. The comparative studies indicated that there are appreciable differences in dynamic rheological properties between the liquid crystals containing different ionic liquid. The lamellar phase and cubic phase formed in bmim-BF_4 system show typical gel-like mechanical spectra and relaxation spectra while the bmim-PF_6 systems exhibit fluidlike viscoelastic property to some extent. The strength of the network of hexagonal phase formed in bmim-BF_4system is clearly stronger than that of the bmim-PF_6 system. All these differences have been analyzed through SAXS data as the different locations of ionic liquids in the liquid crystal phases, that is, bmim-PF_6 is dominantly penetrated between the EO chains of surfactant molecules whereas bmim-BF_4 is mainly located in the water areas of the liquid crystals. References1. Zhongni Wang, et al. J. Coll Inter Sci. 2008, 318: 4052. Zhongni Wang, et al. Langmuir, 2005, 21: 4931.3. Zhongni Wang, et al. J. Solution Chemistry. Accepted.

Adsorption, CMC, and Solubility in Nonionic Biosurfactant Mixtures with SDS and CTAB. K.M. Werts, B.P. Grady, University of Oklahoma, Norman, OK, USA

Some widely-used surfactants are perceived to be harmful to the environment, however their combination of performance+cost makes them very attractive for many applications. Although in some respects not as advantageous as full replacement, partial replacement of these harmful surfactants with biodegradable biosurfactants might be attractive, especially when these systems show better properties than the individual solutions. Solubility, adsorption, surface tension, and critical micelle concentration measurements were taken for different industrial and biosurfactant mole fraction mixtures. The mixtures consist of nonionic biosurfactants (Decanoyl-n-methylglucamine and N-nonyl-b-D-glucopyranoside) and two quite common ionic surfactants (sodium dodecylsulfate and cetyl trimethylammonium bromide). The behavior of these nonionics in mixtures will also be compared to mixture behavior for other more typical nonionics. We are attempting to identify systems where we might see synergistic or otherwise interesting properties in these mixtures.

Solubilization of Nutraceuticals into Reverse Hexagonal Mesophases. Idit Amar-Yuli, Abraham Aserin, Nissim Garti, The Hebrew University of Jerusalem, Jerusalem, Israel

Liquid crystals are widely utilized as model systems to mimic biological processes where the phase behavior of lipids plays a mediating role. In various foods, pharmaceutical and biotechnical applications, the liquid crystalline phases formed by surfactants in an aqueous medium represent useful host systems for drugs and vitamins.Various biologically active food additives are insoluble in neither aqueous nor oil phase and require environmental protection against hydrolysis or oxidation. Liquid crystals meet these requirements mainly due to their high solubilization capacities for hydrophilic, lipophilic and amphiphilic molecules. We report on the solubilization of four bioactive molecules with different polarity, in three reverse hexagonal (HII) systems. The systems were composed of glycerol monooleate (GMO)/tricaprylin/water and two fluid hexagonal systems containing either 2.75 wt% of Transcutol or ethanol as a fourth component. The phase behavior of the phases in the presence of ascorbic acid, ascorbyl palmitate, D-α-tocopherol and D-α-tocopherol acetate were determined by small-angle X-ray scattering and optical microscopy. Differential scanning calorimetry and Fourier-Transform infrared techniques were utilized to follow modifications in the thermal behavior and in the vibrations of different functional groups upon solubilizing the nutraceuticals.

Increasing Oxidative Stability of Lipid Bioactive Compounds in Solid Lipid Nanoparticles (SLN) by Controlling Crystallization with High Melting Lecithin. Thrandur Helgason[1,2], Tarek Awad[2], Kristberg Kristbergsson[1], Eric Decker[2], Julian McClements[2], Jochen Weiss[3], [1]University of Iceland, Reykjavik, Iceland, [2]University of Massachusetts, Amherst, MA, USA, [3]University of Hohenheim, Stuttgart, BW, Germany

Solid lipid nanoparticles, which consist of crystalline lipid particles dispersed in water, can be used to encapsulate bioactive ingredients. However lipid molecules may recrystallize resulting in expulsion of lipid bioactives. Objectives

were to control the crystal structure by engineering the particle interface. β-carotene (2mg/g) was dissolved in tripalmitin at 75°C and mixed (10%w/w) with hot surfactant solution containing high, or low melting lecithin (2.4%w/w) and 0.6% taurodeoxycholate as co-surfactant at pH 7. The solution was homogenized in a microfluidizer at 12000 psi and then cooled to 20°C to induce solidification of the lipid matrix.By using high melting lecithin as a surfactant the crystallization onset temperature changed from 21.18±0.04°C to 30.11±0.28°C, suggesting nucleation from the interface. A high presence of α-subcell structures in the sample stabilized with high melting lecithin suggests that the polymorphic transition was retarded. High melting lecithin preserved the β-carotene better with only 3.9±3.2% breakdown after 11 days of storage compared to 87.9±8.0% breakdown when using the low melting lecithin.This suggests that the use of a surfactant where tails crystallize prior to the lipid matrix may lead to generation of a structure that is better capable of containing the bioactive.

Microemulsion-based Detergency: Cost-effective and Environmentally-friendly Formulations Optimized for High-unsaturated-content Vegetable Oils. T. Phan, J. Harwell, D. Sabatini, University of Oklahoma, Norman, OK, USA

Vegetable oils are among the most difficult oils to remove from fabrics due to the highly hydrophobic nature of triglycerides. With concerns about heart diseases associated with saturated triglyceride intakes, consumers have shifted to high-unsaturated-content vegetable oils. This tendency poses a great challenge to vegetable oil detergency because unsaturated triglycerides are more hydrophobic thus harder to be cleaned by surfactants.The objective of this study is to provide qualitative guidance for surfactant selection for high-unsaturated-content vegetable oil detergency. Effects of extended surfactant structures (chain length, branching, EOs, POs) on IFT and phase behavior will be evaluated. Mixtures of extended surfactants and conventional surfactants, bio-based surfactants and linkers will be also evaluated to formulate cost-effective and environmentally-friendly systems. Detergency tests will be conducted for selected formulations and vegetable oils with varying unsaturated contents. Effects of salinity, surfactant concentration, surfactant ratio on overall and unsaturated triglycerides detergency efficiency will be evaluated. Optimized systems that can provide high detergency efficiency with low salinity and low extended surfactant concentrations will be recommended.

Synthesis, Characterization, and Properties of Anionic Gemini Surfactants having Different Spacer Groups. Rashmi Tyagi, Parul Tyagi, Jaypee Institute of Engineering and Technology, Raghogarh, Guna, Madhya Pradesh, India

Anionic gemini surfactants having different spacer groups have been synthesized. The resulting anionic gemini surfactants were characterized using modern instrumental techniques viz, FT-IR, 1H-NMR and 13C-NMR. In the present study, an attempt has also been made to improve the yield of mono alkyl phosphate, which was used as an intermediate in the synthesis of geminis. These long chain mono alkyl phosphates have effectively been converted to bis (alkyl-phosphates) and subsequently converted to di sodium salts with good yield. Surface active and performance properties of synthesized geminis were also determined.

Admicellar Formation and Adsolubilization of Anionic Extended Surfactants onto Aluminum Oxide. Chodchanok Attaphong[1], Noulkamol Arpornpong[1], Ampira Charoensaeng[1], Sutha Khaodhiar[2], David A. Sabatini[3], [1]National Center of Excellent for Environmental and Hazardous Waste Management (NCE-EHWM), Bangkok, Thailand, [2]Environmental Engineering, Chulalongkorn University, Bangkok, Thailand, [3]School of Civil Engineering and Environmental Science, University of Oklahoma, Norman, OK, USA

Anionic extended surfactant systems are evaluated for making surfactant modified adsorbents. Four types of anionic surfactants, conventional surfactant (SDS), polymerizable surfactants, alkyl propoxylated sulfate surfactants, and alkyl propoxylated ethoxylate carboxilate surfactants were adsorbed on the alumina. Adsorbed admicelles at solid/liquid interface are capable of solubilizing organic solute from aqueous phase known as adsolubilization process. This study evaluated the adsolubilization enhancement of organic solute. In addition, due to surfactant loss from solid surface, desorption potential was determined to evaluate the stability of surfactants adsorbed onto surface. These results provide useful information on surfactant-based surface modification to enhance contaminant remediation and industrial applications.

Effect of Hydrophobic Guest Molecules on the Discontinuous QL Cubic Mesophase and Its Soft Nanoparticles. Rivka Efrat[1], Abraham Aserin[1], Dganit Danino[2], Nissim Garti[1], [1]The Hebrew University of Jerusalem, Casali Institute of Applied Chemistry, Jerusalem, Israel, [2]Technion, Israel Institute of Technology, Department of Biotechnology and Food Engineering and the Russell Berrie Nanotechnology Institute, Haifa, Israel

Hydrophobic bioactive guest molecules were solubilized in the discontinuous cubic mesophase (QL). Their effects on the mesophase structure and thermal behavior and on the formation of soft nanoparticles upon dispersion of the bulk mesophase were studied by several techniques (DSC, SAXS, cryo-TEM, and DLS). The guests were classified into two types: type I molecules (carbamazepine and cholesterol) likely localize in the hydrophobic domains, but close to the hydrophobic-hydrophilic region. They influence both the order of the lipid acyl chains and interactions between lipid headgroups. The inclusion of type I molecules in the mesophase also prevents the formation of soft nanoparticles with long-range internal order upon dispersion. In their presence, only vesicles or sponge-like nanoparticles form. type II molecules (Phytosterols and coenzyme Q10) localize in the hydrophobic domains, where they cannot alter the lipid curvature or transform the QL mesophase into another phase. Moreover, when type II-loaded QL is dispersed, nanoparticles with long-range order and cubic symmetry do form. A model for the growth of the ordered nanoparticles was developed from a series of intermediate structures. It proposes the development of the internal structure by fusion events between bilayer segments.

S&D 1.2: General Cleaning Technologies
Chair(s): M. Ventura, Church & Dwight Co. Inc., USA; and G. van Buskirk, Clorox Services Co., USA

Polymers in Detergent Formulations. Rakesh Trivedi[1], Saurabh Srivastava[2,1], [1]Ambedkar Institute of Technology, Kanpur, UP, India, [2]Oil Technologist Association of India, Kanpur, UP, India

Abstract-:For a long time polymers are being used as an important ingredient to impart specific performance properties in detergent powder and cake formulation. Now days various polymers are available for used in different kind of detergent products. These polymers reduce processing time, cost, and difficulty and shows excellent inhibition of crystal growth and dispersion of precipitates in the cleaning bath. The most important part is that they can be used in different applications such as: automatic dishwashing, powder and liquid fabric wash, laundry additives, industrial and institutional detergents. Current study is based on the performance of cationic polymers in household detergent powder. The detergent powder incorporated with the polymer shows good anti-precipitation, crystal distortion and dispersing properties as compared to detergent without polymers.

CANCELED - Modified Aluminosilicate Gels as Versatile Rheology Modifiers for Household / Personal Care Formulations. Tapashi Sengupta, AMCOL International Corporation, 2870 Forbs Avenue, Hoffman Estates, IL 60192, USA

Layered aluminosilicates have been used over the years to modify the rheology of aqueous systems, as a suspending and shear-thinning agent, emulsion stabilizing agent, and a very cost-effective replacement for synthetic polymers. AMCOL's rheology modifiers span a wide range of products - from the most natural unpurified clay minerals to the highly modified aluminosilicate pregels used in household and personal care formulations. The surface modified aluminosilicates may be both hydrophilic and hydrophobic, depending on the specific application. The hydrophilic surface modified aluminosilicate pregels function as very effective viscosity modifiers for surfactant solutions, microemulsions, macroemulsions, gels, pastes, bleach cleaners over a wide range of pH and electrolyte concentrations. These pregels have excellent shear thinning and thixotropic properties, rendering formulations sprayable with good spray properties and vertical cling resistance. Customized surface modification of AMCOL aluminosilicates make them particularly suitable rheology modifiers for polar, nonpolar, mixed solvents, and complex formulations. AMCOL surface modified aluminosilicates exhibit superior performance over synthetic products available in the market in such difficult to thicken formulations.

CANCELED - Core-Shell Nanoaggregates from Stimuli Responsive Block Copolymers in Aqueous Solutions. P. Bahadur, Veer Narmad South Gujarat University, Surat Gujarat India

This presentation has been canceled.

Inter and Intramolecular Amphiphilic Mixtures as an Optimum Compromise to Enhance Solubilization in Microemulsion. From Winsor Balanced Interaction. J.L. Salager, C. Scorzza, J. Velasquez, M.A. Arandia, A.M. Forgiarini, Universidad de Los Andes, Merida, Venezuela

The solubilization in microemulsion is maximum in a formulation scan when the interactions of the amphiphilic substances adsorbed at interface for the oil and water phases are exactly equilibrated. Improved solubilization performance could be attained by increasing both interactions. This could be reached first by increasing the size of both surfactant groups. However at some point a limit is attained when the surfactant precipitates. A second way to improve the solubilization performance is to use a mixture of amphiphiles, typically a hydrophilic and a lipophilic amphiphiles combination. This technique has also a limit because the more they are unbalanced, the more the mixture components tend to partition into the bulk phases instead of co-adsorbing at interface. The partitioning could be reduced by attaching the parts together, i.e. by forming an intramolecular mixture. This was the basic motivation to build up the so-called extended surfactant structures. Recent advances in the study of such structures are reported, showing that the optimization of their solubilization performance may be carried out by accumulating favorable features such as increasing balanced interactions and mixing slightly different species.

AFTERNOON
S&D 2.1 / EXH 1: Supplier Session
Chair(s): H. Plaumann, BASF Corporation, USA; and M. Robbins, Clorox Co., USA

Replacing Phosphate in ADW Formulations. J. Jefferis, K. Zack, BASF, USA

Phosphate will be removed from consumer ADW formulations by 2010. Experimental Design studies provide systematic cause and effects and are enabling formulators to determine the best approaches to close the performance gap between phosphate and non-phosphate containing products.

Next Generation Oleochemical and Surfactant Technologies. M. Shea, A. Catalano, Chemithon Corporation, Seattle, WA, USA

Chemithon Corporation has established new capabilities to provide value added processes to existing biodiesel facilities, such as distillation, hydrogenation, and ethoxylation, in addition to sulfonation processes. The presentation briefly describes each new process capability and introduces our new global operation based in Singapore - Chemithon International Pte. Ltd.

The Battelle World Detergent Program. F. Pala, Battelle Memorial Institute, USA

For more than 20 years, the Battelle World Detergent Program (BWDP) has provided accurate, quick, and cost-effective compositional analysis of detergent products found throughout the world. The BWDP is a multi-client study that shares the cost of analysis among all program subscribers. An overview of the BWDP, including the analytical capabilities for determining detergent composition and the program database supplied to the clients, will be presented.

Technological Forecasting Helps Us Make Better Decisions!. Jesse Jefferis, Shafeek Razac, Marie Fraties-Block, Heinz Plaumann, BASF Corporation, Wyandotte, MI 48192, USA

We are often involved in forecasting and trend analysis, planning our business growth (or more lately, how things might decline!). This includes such elements as market growth, planning for capital investments, acquisitions and divestitures, examining probabilities for our profitability and Return on Investment.Many times Technological Forecasting is neglected in this analysis. Such forecasting may be based strongly on life cycle analysis: When will our current product offering become obsolete? When is the correct time to undertake an R&D project and bring something new to market? Strategically, do we want to be first to market to "fast-followers"?In this paper, we present a simple approach allowing us to answer some of these questions. The Fisher-Pry model for forecasting has proven useful to us

in a number of areas. A simple explanation of the model, with examples of general interest, are given (growth of home computers and internet access in USA). More pointed examples for the chemical industry are also discussed with a few directly relevant to the Consumer D&C market. The model is fairly simple to use, especially in its linearized form, and gives us information about the rate at which a new product or technology is replacing the old, as well as an estimate time for "half replacement", when the new has successfully replaced half of the old. Problems and limitations of the model are also given.Happy forecasting!

S&D 2: General Surfactants II
Chair(s): S. Adamy, Church & Dwight Co. Inc., USA; and M. Tsumadori, Kao Corporation, Japan

Effect of Hydrophobic Chain on the Surface Active/Performance Properties of Imidazolinium Surfactants. V.K. Tyagi, Divya Bajpai, Harcourt Butler Technological Institute, Kanpur, Uttar Pradesh, India

Imidazoline surfactants belong to the category of cationic surfactants which are now gaining importance due to their varied and numerous industrial applications. Imidazolinium surfactants comprises hydrophilic head group of five membered imidazoline ring and a hydrophobic chain, generally C12-C18 saturated/ unsaturated fatty alkyl group. The present study describes the effect of hydrophobic chain on the surface-active and performance properties of imidazolinium surfactants viz. cmc, surface tension, dispersability, emulsion stability, foaming, softening, rewettability, and detergency.

Effects of Sodium Bicarbonate on Mixed Surfactant Systems. S. Adamy[1], D. DeVece[2], [1]Church & Dwight Co., Inc., Princeton, NJ, USA, [2]The College of New Jersey, Ewing, NJ, USA

Studies on the effects of sodium bicarbonate on mixed surfactant systems containing alkyl sulfates and amine oxides were performed. Non-ideal behavior in the mixed surfactant systems was characterized via calculation of interaction parameters. Values of interaction paramters were found to be influenced by surfactant type and sodium bicarbonate concentrations.

CANCELED - Novel Fabric Bleaching Techniques with Metal Complex Catalysts and Hydrogen Peroxide. Tomonari Suekuni, Yukiko Iwasa, Yosuke Kono, Takayasu Kubozono, Nobuyuki Yamamoto, Lion Corporation, Edogawa-Ku, Tokyo, Japan

Recently, consumers have come to pay much attention to hygiene. Similar trends are also seen in the household product's field, so they have come to expect the functions of removing invisible soil such as odors and bacteria for laundry detergents. Although hydrogen peroxide or a conventional organic bleach activator is utilized to achieve such results, their effect is not necessarily sufficient.Therefore in order to achieve a higher effect, bleach catalysts have been developed in this field. Bleach catalysts can boost the potential of hydrogen peroxide. However too strong an oxidant causes problems such as fabric damage and discoloring when used in laundry detergents. Therefore, the technical issue to develop bleach catalysts is how to obtain a balance between high performance and low fabric damage.In this situation, we succeeded in the development of a novel bleach catalyst for laundry detergents. We determined that our catalyst is effective not only for bleaching food stains but also for decomposing other organic compounds and disinfecting. Meanwhile, we confirmed that our catalyst has no negative effects on fabric.In this report, we will describe some of the unique functions which cannot be achieved by conventional bleach systems and the putative mechanism of stain decomposition.

Screening of Cationic-Anionic Surfactant Interactions Using High Through-put Formulation Robot (HTF-Robot). M. Islam[1], M. Dery[1], J. Speelman[2], A. Wismeijer[2], [1]AkzoNobel, Brewster, NY, USA, [2]AkzoNobel, Deventer, The Netherlands

A total of six anionic and five cationic surfactants were investigated, generating a total of 750 unique blends. These blends were prepared and investigated using the HFT-Robot to create 30 phase diagrams. The data will be presented and discussion will be made in terms of interaction of different types of surfactants.

Adsorption, Adsolubilization and Corresponding AFM Studies for Polymerizable Gemini Surfactant. Emma Asnachinda[1], David Sabatini[2], John O'Haver[3], Sutha Khaodhiar[4], [1]National Center of Excellence for Hazardous Waste Management, Chulalongkorn University, Bangkok, Thailand, [2]Department of Civil Engineering and Environmental Science, University of Oklahoma, Norman, OK, USA, [3]Department of Chemical Engineering, University of Mississippi, Oxford, MS, USA, [4]Department of Environmental Engineering, Chulalongkorn University, Bangkok, Thailand

To mitigate surfactant loss from surfactant-modified adsorbent, polymerization of surfactant has been used. Recently, gemini surfactant was found to enhance the property of solid oxide surface over the single head group conventional surfactant. Corresponding to this finding, polymerizable gemini surfactant was used to evaluate a new genre for surfactant-modified material. It was expected to minimize surfactant losses as well as improve operating characteristics of the surfactant-modified media. The adsorption of polymerizable gemini surfactant and the adsolubilization of organic solute were performed in batch experiments at room temperature (25±2°C), constant pH solution in the range of 6.5-7.5, and electrolyte concentration of 0.001 M NaBr. The adsolubilization of organic solute, styrene, was carried out to evaluate the adsolubilization capacity of polymerizable gemini surfactant with different degree of polarity in admicelles. To extend the studies of adsorption and adsolubilization from bacth experiment, atomic force microscopy (AFM) studies were used to examine the polymerized plane as a surface characterization in order to estimate corresponds to those adsorption and adsolubilization studies.

Characterizing the Non-Idealities of Mixtures of Anionic-Nonionic Surfactants in Surfactant-Oil-Water (SOW) Systems. Edgar Acosta, University of Toronto, Toronto, Ontario, Canada

It is well known that mixtures of anionic and nonionic surfactants typically have critical micelle concentrations lower than the pure surfactants alone. This synergistic effect ? in micelle formation ? is characterized by an interaction parameter β. The nonionic surfactant helps mitigating the same-charge repulsion between anionic surfactant molecules, facilitating their self-assembly in micelles. In microemulsions, however, the effects of adding nonionic surfactants are more complex. This presentation looks at the changes in the curvature of surfactant aggregates (micelles, reverse micelles and bicontinuous systems) in mixtures of anionic and nonionic surfactants. The hydrophilic-lipophilic difference (HLD) equation is used to quantify these changes. It was found that in mixtures of anionic and nonionic surfactants there are two interaction parameters to consider. The first interaction parameter, A1, reflects the charge shielding effect of the nonionic surfactant in anionic-rich surfactant systems. The second interaction parameter, A2, reflects the hydration effects that anionic surfactants introduce when used in nonionic surfactant-rich systems. These parameters are used to describe the phase behavior of limonene microemulsions formulated with binary mixtures of sodium dihexyl sulfosuccinate (SDHS) with nonylphenol ethoxylates and alkyl ethoxylates. These expressions were also used to predict the composition of temperature-insensitive AOT-C12E5-heptane microemulsions. The results of that prediction are in good agreement with experimental data.

TUESDAY

AFTERNOON
S&D 3.1: Industrial Applications of Surfactants
Chair(s): T.-C. Jao, Afton Chemicals, USA; and M. Rosen, Brooklyn College, USA

Impact of Surfactants on Passenger Car Fuel Economy. J.T. Loper, Afton Chemical Corp., Richmond, VA, USA

In recent years there has been growing concern about automobile fuel economy. Government standards such as CAFÉ have required cars to have higher fuel economy. Even modern engine specifications require lubricants to demonstrate fuel efficiency in standardized engine tests. The thickness and frictional characteristics of lubricant films are known to affect the fuel economy properties of oils. These lubricant frictional characteristics include thin-film friction and boundary friction. Thin film friction is the frictional force generated by pushing a fluid between two narrowly separated surfaces. Boundary friction is the frictional force generated when the rubbing surfaces of a machine such as an engine, come in contact. Any frictional force that resists the motion of the surfaces in that machine results in a loss

of efficiency. The additional fuel consumed to counteract these frictional forces translates into a reduction in fuel economy.The choice of surfactants can impact the both the thickness and frictional characteristics of the lubricating oil. The response of surfactants on these frictional characteristics will be presented.

W/O Microemulsions of Vegetable Oils as a Biodiesel Alternative. Linh Do, Thu Nguyen, David Sabatini, University of Oklahoma, Norman, OK, USA

Vegetable oils have been considered as a renewable energy for diesel. Due to high viscosity, use of vegetable oils causes engine durability problems. Microemulsification is a method to reduce vegetable oil viscosities. This method requires no chemical reactions and is easy to implement. In this work, we focused on reverse micellar microemulsions(ME) of vegetable oil/diesel blend using a mixed extended-surfactant and sugar-based(SB) nonionic surfactant system as an alternative to diesel fuel. Extended-surfactants have intermediate propoxylated(PO) and/or ethoxylated(EO) groups inserted between the surfactant molecules. Owing to their unique structures, extended-surfactants enhance solubilization with hydrophobic oils. However, the nonionic characteristics of the EO-PO groups will result in temperature sensitive ME. Thus, non-ionic sugar-based(SB) surfactants was incorporated to form ME fuels. SB surfactants are biorenewable. SB surfactants can be used to formulate temperature insensitive ME since sugar groups do not dehydrate with increasing temperatures. In addition, SB non-ionic surfactants do not contain sulfur which is favorable in fuel properties. We have achieved a stable ME with viscosity comparable to that of diesel. We were also able form temperature nonsensitive ME fuel using SB surfactants. The water solubilization in ME is less than 10% which is acceptable in fuel.

Vegetable Oil Extraction Using Reverse Micellar Microemulsions of Diesel for Biodiesel Application. T. Nguyen[1,2], L. Do[1,2], D. Sabatini[1,2], [1]University of Oklahoma, Norman, OK, USA, [2]Institute for Applied Surfactant Research, Norman, OK, USA

Research has shown that vegetable oils are a feasible substitute for diesel fuel, and short term tests using neat vegetable oils showed promise with results comparable to those of diesel fuel. However, engine problems arise due to the high oil viscosity. In this research the blending of vegetable oil and diesel as a way to reduce the viscosity is done via oil extraction of peanuts using diesel reverse micellar (water-in-oil or W/O) microemulsions (MEs). The advantages of this method include the elimination of the transesterification step required in biodiesel production and less refining steps as compared to those in edible oil extraction. As a result, the extraction solvent will be diesel W/O MEs and the extraction of vegetable oil is based on the â??likes dissolve likesâ? principle. Various extraction parameters are evaluated to optimize the efficiency of peanut oil extraction. The objectives of this research thus include first the formulation of W/O microemulsions with diesel using biosurfactants and biorenewable surfactants and then application of these W/O microemulsions as the extraction solvent. The extracted peanut oil/diesel blends are analyzed for peanut oil/diesel ratio, viscosity, free fatty acid content, acid composition and phosphatides content.

Viscoelastic Surfactants for Oil Recovery. P. Berger, C. Lee, Oil Chem Technologies, Sugar Land, TX USA

This paper will discuss the use of viscoelastic surfactants to recover crude oil. As much as two-thirds of all the oil in subterranean reservoir remains after primary and secondary recovery. This oil is trapped in the microscopic pores of the reservoir rock and cannot be removed without overcoming the strong capillary pressure retaining this oil. It has been found that lowering the interfacial tension (IFT) between injected brine and the trapped oil to values below 1 x 10^{-2} mN/m helps to penetrate these pore spaces.Polymer is added to control the mobility so the injection fluid does not by-pass the oil by seeking paths of least resistance. In many cases polymer cannot be used because of temperature and/or salinity restraints. Certain amphoteric surfactants not only give low IFT against the trapped oil but also increase viscosity of the injection fluid. They are not broken down by shear and they are thixatropic so that their viscosities are very low under high shear and very high under low shear. Thus they are easily injected at the wellhead. In addition their viscosities are reduced when they contact oil but remain high when contacting water. This allows solutions containing these surfactants to preferentially seek out and remove the crude oil.

Adjusting Optimum Salinity of Anionic Micro-emulsions used in Enhanced Oil Recovery with Alcohol Ethoxylates. Charles Hammond, Geoff Russell, Sasol North America Inc., 2201 Old Spanish Trail, Westlake, LA,

USA

In surfactant induced enhanced oil recovery (EOR), there is a need to formulate the surfactant package to give optimum performance at the specific conditions of each oil well (i.e temperature, oil type, salinity, etc.). Anionic surfactants, especially those based on alcohol propoxy sulfates, are showing to have good oil recovery performance for many wells with temperatures < 70°C. Each anionic surfactant, however, has an optimum salinity at which it performs best or creates a Windsor III microemulsion. This study will show that the optimum salinity of alcohol propoxy sulfate anionic surfactants can be significantly shifted to higher or lower salt concentrations by using a non-ionic alcohol ethoxylate as a co-surfactant.

Interaction and Synergism in Surfactant/Water Soluble Polymer Combinations in Boosting Foaming Performance in Home, Personal Care Formulations. Manilal Dahanayake[1], Tobias Futterer[2], Milton J. Rosen [3], [1]Rhodia Inc., Bristol. 350george Patterson Blvd., PA 19007, USA, [2]Rhodia Inc., 51 Science Park Road #04-01/09, The Aries, Singapore Science Park II, Singapore 117586, [3]Surfactant Research Institute, Brooklyn College, CUNY, NY 11210, USA

Some Water soluble polymers both synthetic and natural, are very well known to increase foam stability in surfactant based formulations and have been extensively used in formulating products to enhance esthetic properties in personal care formulations and/or functional properties in industrial applications. However, recent trends in industry for use of " Green Chemistry " in personal care products are growing dramatically. In this respect several cationic and non-ionic guars, with excellent environmental profile and mildness, have been developed. These polymers in addition to providing foam stability are surprisingly capable of enhancing initial foam volumes significantly. For these polymers we have found that improvement in foaming performance is accompanied by decrease in dynamic surface tension, an increase in the dilational elasticity and bulk viscosity. In this paper use of latest techniques to measure surface rheology and the relationship between foaming performance and surface rheological properties will be discussed.

Effect of Nonionic Surfactant Molecular Structure on Cloud Point Extraction of Phenol from Wastewater. P. Taechangam[1], J.F. Scamehorn[2], S. Osuwan[1], T. Rirksomboon[1], [1]Petroleum and Petrochemical College, Chulalongkorn University, Bangkok, Thailand, [2]Institute for Applied Surfactant Research, University of Oklahoma, Norman, OK, USA

Above a temperature known as the cloud point, aqueous solutions of nonionic ethoxylated surfactants separate into two phases: a coacervate phase concentrated in surfactant and a dilute phase with low surfactant concentration. The coacervate phase contains surfactant aggregates which are micelles or micelle-like and will solubilize any organic solutes originally present in the water, resulting in a liquid-liquid extraction known as a cloud point extraction (CPE). Phenol is used as a model pollutant here. In this study, we investigate the effect of surfactant structure on equilibrium CPE parameters for alcohol ethoxylates (AE). Pure, homogeneous surfactants with linear hydrophobes are studied as well as commercial heterogeneous AEs with both linear and branched hydrophobes. The solubilization equilibrium constant is shown to increase linearly with EO number and is unaffected by alkyl carbon number or hydrophobe branching from which we deduce that the phenol is solubilized with the benzene ring at the surface of the micelle core and the hydroxyl group having attractive interactions with the polyethoxylate chains in the palisade layer of the micelle. Guidelines for surfactant selection for CPE of phenol or similar solutes are outlined.

Simultaneous Recovery of Trace Heavy Metals and Surfactants Using Multi-stage Foam Fractionation. Visarut Rujirawanich[1], Sumaeth Chavadej[1], John H. O'Haver[2], [1]The Petroleum and Petrochemical College, Chulalongkorn University, Bangkok, Thailand, [2]Department of Chemical Engineering, The University of Mississippi, Oxford, MS, USA

Due to severe toxicity of heavy metal in environment, removal of heavy metal ions is of particular interest in recent hazardous waste research. Currently, usefulness of available techniques for metal ions removal is limited in case of treating large volumes of industrial wastewater at low metal concentration because of high operating cost. In this study, a multi-stage foam fractionation column using bubble-cap trays was used to recover cadmium and surfactants from

simulated wastewater and the effects of type of surfactants and salinity will be studied. The % recovery and the enrichment ratio of both metal and surfactants were used to evaluate the process performance. The multi-stage foam fractionator was operated at different air flow rates, feed flow rates, surfactant to metal ratio and foam heights in order to determine the effects of operational parameters. When the concentrations of surfactant (sodium dodecyl sulphate) and heavy metal ion (Cd^{2+}) in the feed solution were 257 mg/L and 10 mg/L, the enrichment ratio and the % recovery of Cd^{2+} were 37 and 99.6, respectively. The operating conditions were as follows: 60 L/min of air flow rate; 40 ml/min of feed flow rate; and foam height of 90 cm. The Cd^{2+} concentration in the effluent was lower than 0.05 mg/L.

S&D 3: Bringing Things to Market - Innovation in Detergent Ingredients, Formulation, and Supply Chain
Chair(s): J. Pytel, Stepan Co., USA; and G. Dado, Stepan Co., USA

Engaging the Consumer in the Development and Commercialization of Consumer Products. T. Graham, Church & Dwight Co., Inc., Princeton, NJ, USA

The desire to delight the consumer and gain a competitive edge in the marketplace drives product development. Consumer feedback is integral to the development and maintenance of successful consumer products. A variety of interactive test methods are utilized to gain insight into unmet consumer needs. The size of an opportunity determines the strategy for launch. Home shows and direct-response marketing give critical consumer feedback to help define the probability of success at the next stage of commercialization and drive business decisions such as resource allocation and advertising spending. Label claims, print ads, and TV commercials aim to address the consumerâ??s needs by targeting their most common grievances with enthusiasm while being substantiated by real data. These claims are visually communicated through â??demosâ? by trained personalities and product stewards at special events and through advertising (e.g. infomercials). Advertising is a culmination of R&D and Marketing teamwork to support product launches. After launch, the consumerâ??s response is investigated (actively or passively) and used to make product improvements, identify line extensions, and to define further unmet needs. Hence, the product market is expanded through an iterative process.

Challenges to Innovation in the Surfactants Market. G.P. Dado, Stepan Company, Northfield, IL, USA

While many definitions may be found, the term "innovation" can be regarded as the successful implementation of something new. In the surfactants market, changes in customer preferences and needs, raw material economics, and regulatory requirements can be significant drivers for change. The challenge to innovating is then two-fold; identification of the "new" that can address the changing needs of the market place AND successful implementation of this "new". In this presentation, some of the hurdles and challenges to innovation in the surfactant market will be discussed from the perspective of a surfactant manufacturer.

Historical Perspective of Surfactants based on Fatty Acids: From Potts to the Present. Dale Steichen, Maurice Dery, Akzo Nobel Surface Chemistry, Brewster, NY, USA

The roots of all fatty acid based surfactants can be traced back to the pioneering efforts of the Armour meat packing operations and the need to develop uses for the by-products from the food side of the business. In the 1920's Armour established a research laboratory at the Chicago StockYards to expand upon and find new uses for the by-products from the meat packing industry. During the 1930's the first commercial fatty acid fractionation unit was commercialized by Dr. Ralph Potts of Armour Chemical thus making pure fatty acids available on a commercial scale. Ten years later fatty amines were being produced by the nitrile route on a commercial scale. The first commercial application of fatty amines (ca. 1939) was for the beneficiation (separation by flotation) of potash. The first successful commercial process to prepare quaternary ammonium compounds appeared in the 1940's. Dialkyl quaternaries were soon to be very desirable for use in organo modified clays critical in drilling muds. Fabric softeners were developed in the late 1940's as a response to the industries change to synthetic detergents. Growth throughout the years was steady resulting in the current demand for cationic surfactants at over 330 M tons with an estimated economic value of close to a billion dollars.

In-Silico Approach to Innovations in the Laundry Market. R. Olmedo, DETERTEC, Quito, Ecuador

In the laundry products industry, business competition is fierce, with an accelerated commoditisation of products and services, increasing price wars, and shrinking profit margins. R&D teams are pressured to accelerate their pace of innovations to stay ahead, but with different cost structures, being collaborative with external sources and compelled to be more consumer-relevant. There is an urgency to innovate the way R&D innovates.The paper describes the way relevant consumer sensory experiences are capable to be included upstream in the innovation process using computer-based technologies. A novel in silico approach rests on a mixture of tabulated data computations from new photonic devices, customised mathematical models of consumer?s perceptions, and simulation of concatenated events that include changes on materials surfaces and how they are perceived in different visual realities. The in silico technologies to experiment virtually, offer unparalleled advantages against conventional costly and lengthy in vivo and in vitro alternatives, and additionally provide a significant return on investment.Scripting and numerical capabilities as well as interactive 3D graphical and non-linear modelling features are clearly exemplified and presented as the key affordable tools of the new technologies to innovate.

CANCELED - Improving Enzymatic Stain Removal in Laundry Detergents at Low Wash Temperatures. J. Billman, Genencor, A Danisco Division, Palo Alto, CA USA

The trend to lower wash temperatures presents a significant challenge for the detergent formulators as consumers desire equivalent cleaning at ever lower wash temperatures. Innovative detergent ingredients are required to maintain the current high levels of performance as the wash temperature falls. In this presentation a process for bringing to market new enzyme molecules that meet this challenge is presented. The discovery, redesign, improvement, and production of new enzymes that enable effective cleaning at reduced wash temperatures is reviewed. The results of such protein engineering and manufacturing capability enable the continuing reduction in wash temperature without loss of cleaning performance. Examples of engineered enzymes with improved low temperature wash performance are presented.

New Development for Detergents and Cleaners. M. Busby, P. Varineau, Dow Chemical, USA

Dow has introduced a new line of nonionic surfactants based on the 2-ethylhexyl hydrophobe. Block alkoxylation with propylene oxide or butylene oxide extends 2-ethylhexyl alcohol into the detergent range. Ethoxylation of this extended alcohol produces nonionic surfactants with advantaged detergent behavior. These surfactants demonstrate unique surface-active properties such as surface tension reduction, wetting, emulsifying, and low CMC. In addition to surfactancy, their structure also makes them effective coupling agents. They effectively couple difficult materials such as d-limonene, and they stabilize other solvents and help to solubilize difficult to remove soils. These surfactants performed as effective substitutes for alkylphenol ethoxylates, and they also showed improved stability compared to traditional primary alcohol ethoxylates. Cleaning formulations incorporating these new surfactants have been prepared and tested, and the results will be presented.

Ternary Surfactant System for Hard Surface Cleaning. S. Gross, A. Kvecher, V. Lazarowitz, T. Morris, Cognis Corporation, Ambler, PA, USA

Ready to use All-Purpose Spray Cleaners usually contain alkaline builders, surfactants and solvents. This three-component system is known as the â??performance triangleâ?. It is generally known by one skilled in the art of formulation, that if one component is removed from the performance triangle, the hard surface cleaning ability of the composition is compromised. It is, however, often desirable to reduce or remove the solvent or volatile organic compound (V.O.C.) content of consumer cleaning products not only to comply with legislated V.O.C. limits in some states but also to help reduce the negative effects of V.O.Câ??s in the atmosphere, ie ozone depletion, global warming. It is also often desirable to reduce or remove the alkali content of consumer cleaning products not only to reduce formulation raw material costs, but to improve the overall safety of the formulation in terms of corrosivity, skin irritation and compatibility with a wider variety of hard surfaces. A challenge for the formulator has been to maintain good hard surface detergency on oily soils without the use V.O.C.â??s or alkaline builders. A concentrated ternary surfactant mixture was developed which exhibits remarkable hard surface detergency, without the use of volatile solvents or alkaline builders, upon dilution in water.

WEDNESDAY

MORNING

S&D 4: Regulatory Issues

Chair(s): M. Dery, Akzo Nobel Surface Chemistry, USA; and P. Ferm, Akzo Nobel Chemicals Inc., USA

Consumer Product Ingredient Communication: Industry's Proactive Approach to a Complex Issue. M. Radecki, The Soap and Detergent Association, Washington, DC, USA

The abstract will describe a model developed by The Soap and Detergent Association (SDA) and its association partners for providing consumers with ingredient information about cleaning, air care, automotive and polishes and floor maintenance products. It will address the complexities involved with meeting consumer demands for ingredient information while protecting trade secrets.

Selection Pressure: The Impact of Regulations on the Cosmetic Industry. D. Bower, Akzo Nobel SPG, LLC, Bridgewater, NJ, USA

The chemical industry is subject to a variety of regulations, many of which were enacted in response to specific events. Chemical users responded by selecting different products, and chemical manufacturers responded through product rationalization and process improvements. This interaction of regulations and product design can be viewed as an evolutionary process. In this context, the current status of some wide-reaching regulations affecting the chemical and cosmetics industries will be discussed, along with the implications of these regulations on the evolution of the industry as a whole.

1,4 Dioxane—A Current Topic for Household Detergent and Personal Care Formulators. K.L. Matheson[1], G. Russell[1], B. MacArthur[2], W.B. Sheats[2], [1]Sasol North America, Westlake, LA, USA, [2]Chemithon, Seattle, WA, USA

The presence of 1,4 Dioxane in household detergent and personal care formulations is a product safety topic which has re-emerged after many years. This presentation will focus on alcohol ethoxylates and alcohol ethoxy sulfates in an attempt to clear up some misconceptions about 1,4 dioxane, where it comes from, and how it is formed. Furthermore we will discuss how it can be minimized in alcohol ethoxy sulfates through the use of modern processing equipment, proper sulfation and neutralization procedures, and the appropriate choice of sulfation feedstock.

Update on Zero P Regulations for Autodish Formulations. R. Sedlak, The Soap and Detergent Association, Washington, DC, USA

The presentation will be a review of the status of legislation restricting the maximum phosphorus weight in household automatic dishwashing detergents to 0.5% effective July 1, 2010.Passage of such legislation was made a Soap and Detergent Association legislative priority in 2006.

New Biodegradable Bio-Polymer for Scale Control and Dispersion in Detergents. Klin Rodrigues, Allen Carrier, Jerome Mercanton, Dallas Hetherington, Akzo Nobel, Chicago, IL, USA

AkzoNobel has developed a new developmental, biodegradable biopolymer technology for the detergents market. Based upon the combination of selected polysaccharides and synthetic monomers, the polymers based on this technology biodegrade in the OECD 301 test and prevent scale in detergent formulations such as automatic dishwash systems. This new technology is different from previous biopolymers attempts, such that it promises to be a cost effective approach to a more sustainable future.The paper will present detail on the molecule, its performance in automatic dish detergents and environmental performance.

The Changing Landscape of Chemical Regulations and the Soap and Detergent Industry. M.H. Wolf, C.A.M. Bondi, Product Sustainability & Authenticity, Seventh Generation, Inc., USA

Increased interest in protecting the environment and human health through reducing toxic chemical exposure in conjunction with the green movement has resulted in a shift in industry focus and increased demand for regulation of chemicals. In response, several pieces of legislation have been initiated to promote or require the use in greener chemistries in soap and detergent products. This paper will describe recently implemented and currently proposed regulations and their implications for the soap and detergent industry as a whole.

Environmental Life Cycle Thinking Based Tools as Support for Decision Making within AkzoNobel. T. Boren, AkzoNobel Technology & Engineering, Göteborg, Sweden

The global economy continues to grow in a natural resource constrained world. This is reflected in increased raw material prices, emission fees, and environmentally conscious customers and investors. For corporations it is therefore vital for their future success to ensure that value creation and lowering the impact on the environment goes hand in hand. i.e. to become more eco-efficient. To manage the business risks and opportunities that these constraints imply it is essential to have a toolkit in place that guide decision makers by letting them make informed decisions.This paper describes the life cycle thinking based tools Eco-Efficiency Analysis (EEA), Life Cycle Assessment (LCA) and carbon footprint assessment, and gives an account of how these are applied in all functions of AkzoNobel. Eco-efficiency analysis (EEA) is a tool that implements the concept of eco-efficiency into the daily operations of a business by integrating Life Cycle Costing (LCC) and Life Cycle Analysis (LCA). LCA analyses products from a holistic environmental impact perspective, whereas carbon footprint assessments only generate indications of products' impacts on climate change. Carbon footprint assessment is based on LCA, and therefore an EEA and a LCA also generates the carbon footprint of the studied products. These tools help decision makers in making environmentally and financially informed decisions.As an illustrative example of how LCA can be applied to compare the environmental profiles of different solutions for delivering the same customer benefit, an account is given of the main results of a LCA of synthetic vs hybrid polymers. These polymers are used as co-builders in automatic dishwashing and laundry detergents. The synthetic polymer is based on non-renewable raw materials whereas the hybrid technology mainly is based on maltodextrine, a derivative of corn starch, and hence a renewable raw material.The results of the LCA indicates that the hybrid technology results in significantly lower emissions of greenhouse gases and less use of fossil energy resources, compared to the synthetic counterpart. The main reason for this is that the production of the hybrid polymer requires fewer inputs of energy intensive raw materials. On the other hand, the hybrid technology results in increased emissions of eutrophicating substances and appropriation of farm land, since there is an agricultural stage involved in the production of this polymer. However, from a total environmental impact perspective the hybrid technology performs significantly better according to several different sets of environmental evaluation criteria.

BIO 4 / S&D 4.1: Biobased Surfactants
Chair(s): D. Hayes, University of Tennessee, USA; D. Solaiman, USDA, ARS, ERRC, USA; and G.A. Smith, Huntsman Performance Products, USA

Improved Poly(3-Hydroxybutyrate) Synthesis from Glycerol Substrates and the Effect of Sophorolipid Addition on Physical Properties. R.D. Ashby, D.K.Y. Solaiman, USDA, ARS, ERRC, Wyndmoor, PA USA

As biodiesel gains a larger market share, glycerol is produced in ever-increasing quantities as a co-product from chemical transesterification reactions. Our past work showed that by using glycerol as a fermentation feedstock, both bacterial storage polymers (*i.e.*, poly(hydroxyalkanoates), PHA) and microbial glycolipids (*i.e.*, sophorolipids, SLs) can be produced. Poly(3-hydroxybutyrate) (PHB) can be synthesized by a strain of *Pseudomonas oleovorans* from glycerol. Presently, we have attained maximum PHB yields of 1.3 g/L using 10-L fed-batch fermentations with a 2% initial glycerol concentration. This is a 117% increase compared to previous shake flask cultures. Sophorolipids possess surfactant properties and have several potential applications including in cleaning and cosmetic formulations. By adding SLs to solution cast PHB polymer films, SLs acted to reduce tensile strength, elongation and modulus of the polymer films by modifying film surface and porosity. SEM of the PHB:SL composite films revealed that SL addition caused a dimpled surface topography, and the size of the dimples was related to the concentration of SL added to the matrix. In addition, increased concentrations of SL increased film porosity thus providing potential for slow release applications.

Rhamnolipid Production by Denitrifying *Pseudomonas aeruginosa*. Lu-Kwang Ju, Neissa M. Pinzon, Maysam Sodagari, The University of Akron, Akron, OH, USA

Rhamnolipid biosurfactants have various industrial, environmental, and medical applications. Though commonly synthesized by Pseudomonas aeruginosa, rhamnolipids are expensive to produce due to the highly foaming nature and complex metabolic regulations involved. To employ high cell concentrations in the bioreactors while avoiding the excessive foaming associated with aeration, rhamnolipid production by denitrifying P. aeruginosa has been investigated. The studies so far have confirmed the feasibility of this approach but also identified several new challenges that are not encountered in common aerobic or anaerobic (fermentative) bioprocesses. While nitrate is highly water soluble for easy delivery to cells, online monitoring of the nitrate concentration in broth is not available. Methods need to be developed for enabling nitrate supplementation to match the varying cellular denitrification rate. In this presentation, we will summarize what we have learned, including the online NAD(P)H fluorescence profiles corresponding to nitrate consumption. With a newly isolated strain under the denitrifying condition, we also observed the excessive production of metabolites (not rhamnolipids or alginate) that made the broth extremely viscous. Characterization and, if successful, identification of the responsible metabolite(s) will also be presented.

Glycerin Oleate Ethoxylates: Physical Chemical and Performance Properties. George A. Smith, Prakasha Anantaneni, Patrick Weaver, Huntsman Performance Products, USA

There is a growing demand for cleaning products based on natural ingredients. The general public perception is natural ingredients pose less risk to human safety and better for the environment. There are also growing concerns about ingredients based on palm and coconut due to destruction of the rain forest and loss of biodiversity. Natural based surfactants derived from locally grown crops such as soybean, corn and canola could be of considerable interest in the North American detergent market.This paper will discuss the preparation of glycerin oleate ethoxylates (GOE) and their physiochemical and performance properties in detergent applications. Glycerin oleate can be prepared several different ways. Reacting fatty acids or methyl esters with glycerin using a base catalyst is probably the most common production scheme but leads to a complex mixture of mono, di and triglycerides. It is possible to prepare pure monoglycerides by reacting glycerin with acetone, followed by direct esterification and removal of the acetal protecting group but this process is expensive and difficult to scale to the large quantities required for the detergent market. We have found that reacting soybean oil with excess glycerin under base conditions followed by high temperature phase separation produces reasonably pure glycerin mono oleate (GMO) in good yields. GMO can not be ethoxylated using a conventional base catalyst. The catalyst hydrolyzes the ester bond to produce fatty acid and glycerin. To avoid the hydrolysis reaction, GMO can be ethoxylated using a calcium based catalyst. The catalyst adds ethylene oxide of the primary and secondary hydroxyl groups and inserts EO into the ester functionality. The surface properties of glycerin oleate ethoxylates (GOE) was compared to convention alcohol ethoxylates. At the same degree of ethoxylation, GOEs have a lower CMC, cloud point and foam potential than LAEs based on midcut alcohol due to the longer alkyl chain length. GOEs show surface behavior similar to LAEs. Surface and interfacial tension increase with increasing degree of ethoxylation. GOEs show similar detergency to LAEs in single surfactant and multi-component systems.

New Type of Vegetable Oil Ethoxylates for Detergent Application. Raymond W. Cen, Prakasha Anataneni, George A. Smith, Patrick L. Weaver, Huntsman Corporation, 8600 Gosling Rd, The Woodlands, TX 77381, USA

Our Quest for plant-based surfactants continue. We have synthesized a new type of vegetable oil ethoxylates (EVOEs) by reacting epoxidized vegetable oils with EO and/or PO through a ring opening mechanism. EVOEs were found retaining a triglyceride structure and exhibit good surfactant perperties. EVOEs are cost effective for detergent and other HI&I applications.This presentaition will cover surface properties of EVOEs and compare them with those from methyl ester ethoxylates (MEE) and others. Several applications in detergent and hard surface cleaning are also discussed.This new type of vegetable oil ethoxylates can be manufactured cost effectively. So far they exhibit MEE-like performance there a viable choice for HI&I industry.

Biobased Surfactants and Emulsifiers with Antimicrobial Properties. Hans J. Altenbach, Rachid Ihizane, Bernd Jakob, Karsten Lange, Sukhendu Nandi, Manfred P. Schneider, Bergische Universitaet Wuppertal, Wuppertal, Germany

Agricultural crops provide a considerable reservoir of useful and low cost raw materials like fats and oils, plant proteins and carbohydrates. By selective combination of their molecular constituents (e.g. fatty acids, glycerol, amino acids, saccharides) a wide variety of surface active materials can be prepared, all of them - due to their molecular constitution - being potentially highly biodegradable.In an attempt to acylate citric acid for the production of oil soluble derivatives we recently discovered that hydroxy carboxylic acids such as citric acid, malic acid and tartaric acid can be converted in one step and quantitatively into the corresponding O-acylated anhydrides, excellent electrophiles for ring opening reactions with the above nucleophiles from renewable resources, such as glycerol, sugar alcohols, amino acids and various carbohydrates including glucosamine. Next to novel surface active products- including gemini surfactants- several of the thus resulting molecules show additional benefits such as antibacterial properties and are thus potentially useful as multifunctional emulsifiers in cosmetics and food technology.The lecture will describe recent developments regarding novel combination products based on the above hydroxy carboxylic acids.

CANCELED - Characterization and Application of Methyl Ester Sulfonate Powder. Masahiko Matsubara, Yutaka Abe, Hiroyuki Masui, Kensuke Itakura, Ryoji Yasue, Tsutomu Ishikawa, Lion Corporation, Edogawa-Ku, Tokyo, Japan

A surfactant, Methyl Ester Sulfonate(MES) derived from natural fats and oils, shows high detergency at low concentration in hard water, and also has excellent biodegradability. MES is expected to be alternate surfactant to linear alkylbenzene sulfonate(LAS), because MES is an environment-friendly feedstock of surfactant produced from carbon-neutral vegetable oil. Until now, MES mixed detergent is mainly formulated with paste or dilute solution of MES. But these types of MES are more difficult to handle than other surfactant in the points of delivering MES to factory and mixing procedure into formulation. On the other hand, a highly-concentrated MES powder is interested in as a delivery form which can be directly mixed to powder detergent by dry-blend. But there is no detailed report about characters of MES powder and features of MES blended detergent. MES powder in laundry powder detergent shows good dispersibility, solubility and detergency. In this presentation, details of characterization of MES powder will be described. In addition, the detergents produced from other MES forms are compared to that including new MES powder in its properties and detergency. Furthermore, various factors which affect solubility and detergency will be reported.

Characterization and Application of Methyl Ester Ethoxylate. Hiroaki Shindo, Ryo Hyodo, Megumi Sadaie, Takahiro Okamoto, Hiromitu Takaoka, Lion Corporation, Edogawaku, Tokyo, Japan

In our previous report, we showed that Methyl Ester Ethoxylate (MEE) had good surfactant properties such as foaming, solubilization and wettability.Moreover, MEE showed good skin compatibility for hemolytic activity and environmentally-friendly because of good biodegradability. In this report, we found that laundry detergent including MEE as main surfactant has good detergency for sebum.And MEE has the advantage in the foam control, and in the low amount of residual surfactant on the clothes.As a result of good rinsing ability, MEE based detergent was able to reduce total volume of water consumption during the washing process.We would like to report these experimental results and discuss the mechanism.

Solvent-free Enzymatic Synthesis of Saccharide-fatty Acid Ester Surfactants: Bioreactor Design and Role of Supersaturated Solutions. Y. Ran, S.H. Pyo, D.G. Hayes, University of Tennessee, Knoxville, TN USA

Saccharide-fatty acid esters, biodegradable, biocompatible and biobased surfactants and value added products, were synthesized under low-water and solvent-free conditions at 65C in stirredbatchmode and using several different bioreactor systems that employed immobilized Rhizomucormiehei lipase (Lipozyme® IM, Novozymes, Franklinton, NC, USA) at 65C. The environmentally friendly approach, which takes advantage of the enhanced miscibility of acyl donor and acceptorsubstrates in the presence of ester, yields 80-85% ester and strong selectivity toward monoesters, a technical-grade biobased surfactant product that does not require further downstream purification. This presentation will focus upon the development and performance of bioreactor systems for their synthesis. Bioreactor systems that contained a packed column containing saccharide crystals and silica gel for delivery of saccharide provided similar yields to batch-mode reactions, but 3-fold lower rates. Subsequent experiments demonstrated the stirred-tank batch-mode bioreactor systems produced several-fold higher apparent saccharide concentrations due to the formation of

stable ~100 micron-sized suspensions of saccharide crystals in solvent-free media compared to the concentrations yielded by the desorption column in the bioreactor systems.

Surfactants and Detergents Posters

Chair(s): M. Wint, Access Business Group Intl. LLC, USA

Thermodynamics of Mixed Anionic/Nonionic Surfactant Adsorbtion on Alumina.
J.J Lopata, K.M. Werts, J.F. Scamehorn, J.H. Harwell, B.P. Grady, University of Oklahoma, Norman, OK, USA

The adsorption of sodium dodecyl sulfate and a polyethoxylated nonylphenol, and well defined mixtures thereof, was measured on gamma alumina. A pseudo-phase separation model to describe mixed anionic/nonionic admicelle (adsorbed surfactant aggregate) formation was developed, analogous to the pseudo-phase separation model frequently used to describe mixed micelle formation. In this model, regular solution theory was used to describe the anionic/nonionic surfactant interactions in the mixed admicelle and a patch-wise adsorption model was used to describe surfactant adsorption on a heterogeneous solid surface. The formation of mixed anionic/nonionic admicelles in the absence of micelles was accurately described by regular solution theory; mixed admicelle formation exhibited stronger negative deviations from ideality than mixed micelle formation. An adequate description of mixed anionic/nonionic admicelle formation in the presence of mixed micelles was obtained through a simultaneous solution of the pseudo-phase separation models for mixed admicelle and mixed micelle formation, and the appropriate mass balance equations. Anionic/nonionic mixed admicelle formation in the presence of mixed micelles was shown to occur at approximately a 1:1 anionic/nonionic mole ratio throughout adsorption Regions II and III.

Electrostatic Binding Among Equilibrating 2-D and 3-D Self-Assemblies.
L. Shi, F.M. Menger, Emory University, Atlanta, GA, USA

Six organic additives, each bearing a different number of anionic charges, were added to a large excess of cationic surfactant (dodecyltrimethylammonium bromide, DTAB). The surface-tension vs. log [DTAB] plot for solutions containing DTAB/trianion = 15:1 showed an abrupt break (routinely taken as the critical micelle concentration, CMC) at 2.9 mM. This constitutes a 5-fold decrease compared with a CMC of 15 mM for pure aqueous DTAB. There is a 10-fold decrease in the break-point concentration caused by a mere 3 mol-% of hexanion. Corresponding CMC values from DTAB/trianion mixtures, measured by both conductivity and diffusion-NMR, gave normal values of 14 mM. The unusual discrepancy between the CMC based on surface tension and on the two ?bulk? methods was attributed to saturation of the air/water interface by a DTAB/trianion complex far below the concentration at which the micelles form. Thus, the sharp break seen in surface-tension ?CMC plots? need not in fact attest to actual micelle formation as is almost universally assumed in colloid chemistry.

Improved Odor Profile for Selected Methosulfate Quaternaries.
E. Band, W. Joyce, Akzo Nobel Surface Chemistry LLC, Brewster, NY USA

In the synthesis of certain quaternary ammonium methosulfate surfactants odor can be an issue. The prinicipal cause of odor generation has been identified and a method of eliminating the odor during the synthetic process has been established.

Synthesis and Characterization of Lauryl Trimethyl Ammoniums.
Baocai Xu, Zhiqiang Qu, Jinhuan Shui, Yawen Zhou, Fu Han, School of Chemical and Environmental Engineering, Beijing Technology & Business University, Beijing , P.R. China

It is well know that quaternary surfactants possess fine properties and extensive utilities. But in the synthesis research of quaternary surfactants, the structure diversifying at hydrophobic part is always concerned. And quaternary ammonium salts are usually synthesized by using alkyl halides as alkylating agents, which inevitably contaminate the environment and bring toxicity to the target products. The development of green chemistry has made it a prime task

that using green raw materials in the synthesis of quaternary ammonium salts. As new green chemical material, dimethyl carbonate can react as carbonylating agent, esterifying agent, methylating agent, and so on , Herein, lauryl trimethyl ammonium mono-methyl carbonate 1 was prepared by using dimethyl carbonat as alkylating agent and lauryl dimethyl amine as starting material. Then, the mono-methyl carbonate 1 was reacted with formic acid, acetic acid and lactic acid respectively to afford the corresponding quaternary ammonium salts: lauryl trimethyl ammonium formate 2a, lauryl trimethyl ammonium acetate 2b and lauryl trimethyl ammonium lactate 2c.The structures of these compounds were confirmed by IR, 1H NMR, GC-MS and MS.

Potential Benefits of Aluminosilicates as Partial Replacement for Sodium Sulfate in Powder Detergent Formulations.
Carolina Rojas, Steve Azzarello, Amcol International Corp., Hoffman Estates, IL, USA

A thorough study was conducted to identify new potential benefits of aluminosilicates as value-added ingredients in powdered laundry detergents. Aluminosilicates are layered crystalline minerals with unique properties. Their colloidal dimensions and disk-like shape confer them large surface area while their electricallycharged surfaces with adsorbed exchangeable cations make them reactive chemically. Thus, aluminosilicates are useful additives in many applications; low levels of aluminosilicates are used in detergents to achieve fabric care benefits. Sodium sulfate is regarded as relatively inert filler of powdered detergents accounting for up to 50% of the formulation. The lower bulk density of aluminosilicates makes them attractive filler candidates. This work therefore evaluated the effects of partially replacing the sodium sulfate by aluminosilicates in detergent formulations, while giving some insight into the physical-chemical interactions of this complex material with the other ingredients. Phenomena such as electrostatic deposition on hydrophilic surfaces and sequestration of divalent ions during the detergency process were considered. Several additional advantages of formulating with aluminosilicates were demonstrated, such as fragrance longevity, softening-through-the-wash and fabric care, flowaid and anti-caking, and absorption of extra-water. While some of these attributes werealready known, others had remained unexplored. Furthermore, appropriate dosages of aluminosilicates were determined in order to obtain these benefits

Surface Active and Performance Properties of Double Chain Surfactants having Ethylene Spacer.
V.K. Tyagi, D. Shukla, Harcourt Butler Technological Institute, Kanpur, Uttar Pradesh, India

A series of anionic geminis were prepared in two steps by using different fatty alcohols. The chemical structure of the synthesized geminis were confirmed by FT-IR, 1HNMR, 13C NMR spectrum and elemental analysis. The surface active and performance properties of these surfactants (LG-2, DG-2, CG-2) were investigated. The surface tension of these surfactants was found to be 28.7, 26.4, and 23.9mN/m and critical micelle concentration was 0.15, 0.63, 1.9 mmole, respectively. The performance properties like foaming, wetting, emulsion stability and detergency were also evaluated using hard water. The results of the present study revealed that increase in the hydrophobic length of surfactants increased the surface activity of surfactants. It was also found that LG-2 had much better foaming, emulsion stability and detergency as compared to DG-2, CG-2 geminis.

The Effect of Electrolytes on the Interaction of C.I. Reactive Orange 16 -Dodecylpyridinium Chloride.
Halide Akbas, Melike Aydemir, Trakya University, Faculty of Science and Letter, Department of Chemistry, Edirne, Turkey

In the present study, tensiometry has been used to investigate the effect of electrolytes on the interaction of an anionic dye C.I. Reactive Orange 16 (RO16) with a cationic surfactant dodecylpyridinium chloride (DPC) in aqueous submicellar solution at certain temperature. The interaction of RO16 with DPC results a change on the values of surface tension. This change is due to the ion-pair complex formed by the dye and the surfactant molecules. This complex is stable at ambient temperature but unstable with addition of electrolytes. Electrolyte addition to dye-surfactant solution causes a change in absorption value and this change is depending on amount of electrolyte added to solution and surfactant concentrations.NaCl, NaBr, Na2SO4, KCl, KBr, K2SO4 and CaCl2 were used as electrolytes. In this study, the electrolyte cations cause an increase of the absorbance of DPC-RO16 ion-pair complex in the following: Ca+2 > Na+ > K+.. The electrolyte anions have a much smaller effect on these values than the cations and have in the following order: Br- > Cl- > SO4- in the lower electrolyte concentrations. This order may be changeable in the higher concentration. The surface tension of solutions has been measured by the ring method employing a Du

Nouy tensiometer (Kruss K6).

Synthesis, Characterization, and Properties of Tallow Fatty Acids Based Esteramide Quats.
V.K. Tyagi, S. Mishra, Harcourt Butler Technological Institute, Kanpur, Uttar Pradesh, India

A number of amidoester quats have been synthesized from various fatty materials and studied for their softening. The present research paper explores the synthesis of esteramide quat from tallow fatty acids and 1(2-hydroxyethyl piperazine). The instrumental techniques, viz. FT-IR, 1H-NMR and 13C-NMR verified the esterification and subsequent quaternization of the obtained esteramide. Cationic content of synthesized ester quats were also estimated. The resulting quats were also studied for their surface active as well as performance properties viz, surface tension, interfacial tension, cmc (critical micelle concentration), emulsion stability, dispersing power, fabric softening and rewettability.

Impact of Chromatographically Purified Surfactants on the Oxidative Stability of Pharmaceuticals.
S. Ellis, S. Rumbelow, N. Langley, Croda, Inc., Edison, NJ, USA

Surfactants are increasingly becoming more important in the field of pharmaceuticals as excipients in all major routes of drug administration. It is suspected that impurities may react with the active pharmaceutical ingredient (API), thereby affecting its stability in pharmaceutical formulations. The impact of purification of three common surfactants (Polysorbate 80, Dimethyl isosorbide and PEG 400) upon the stability of Benzocaine, a common topical analgesic, was investigated under accelerated storage conditions. Benzocaine stability was monitored by RP-HPLC in which both the loss of benzocaine concentration and the concomitant increase of by-products was observed. The degree of degradation in purified surfactants was considerably less than their unpurified counterparts. In some cases these differences were evident after only four weeks storage at 50^{o}C. It is suspected that these observed differences in stability can be attributed to the presence of higher levels of known oxidants in the unpurified products. This investigation demonstrates how the use of chromatographically purified surfactants can ensure effective delivery of actives by minimising API interactions with the excipient.

Zemea® Propanediol: A New Bio-derived Glycol for Household Cleaning and Liquid Detergent Applications.
P. Colombo, G. Fenyvesi, R. Miller, D.W. Wood, DuPont Tate & Lyle Bio Products LLC, Wilmington, DE, USA

Zemea® propanediol (bio-derived 1,3-propanediol) is a unique offering from DuPont Tate & Lyle Bio Products and manufactured via a proprietary fermentation route. Zemea® propanediol is the perfect high purity glycol for formulations where non-petroleum based ingredients are desired. Zemea® propanediol has been successfully evaluated as a replacement for propylene glycol (1,2-propanediol) in household cleaning and liquid detergent applications. Liquid detergent formulations exhibited excellent cloud point, very good stability, improved foaming, enhanced rheology effects, require less salt to adjust viscosity, and demonstrated soil and stain removal performance similar to propylene glycol formulations. Carpet and rug cleaning formulations showed very high stability, and soil and stain removal performance similar to propylene glycol formulations. This poster will also discuss additional studies demonstrating improved enzyme activity, effective moisturization, lack of skin irritation and sensitization, and 100% bio-based content determined by ASTM D6866 standard. Formulators looking for non-petroleum based ingredients can utilize Zemea®, the first DfE-screened solvent to be listed in CleanGredients®.

Influence of Environmental Stresses on Stability of Antimicrobial Delivery System of Eugenol Encapsulated in Ionic-Nonionic Mixed Micelles.
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Eugenol-loaded micelles have been investigated as novel preseratives to destroy of pathogens in biofilms. However, stability of eugenol-loaded cationic micelles under environmental stresses has not been studied. The purpose of this study was to investigate the influence of environmental stresses on the stability of eugenol-loaded nonionic (surfynol 485W, S485), ionic (sodium dodecyl sulfate, SDS), and ionic-nonionic mixed micelles under environmental

stresses.Eugenol encapsulated in S485 micelles were stable at all pH and salt concentrations, yet were unstable at temperatures >60°C. Eugenol encapsulated in SDS micelles was stable at all pH, NaCl concentrations, temperatures, yet was unstable at CaCl2 (>25mM). The ζ-potential of the SDS particles was strongly negative at acidic pH (e.g., -82 and -80 mV at pH 3 and 3.5, respectively), but became much less negative under other conditions. The ζ-potential of the particles present within the mixed S485-SDS micelles was -7 mV and was stable at high pH, temperature and salts. This suggests that the mixed S485-SDS micelles were more stable than the SDS micelles alone. Results suggest that the combination of S485 and SDS leads to formation of ionic-nonionic stable antimicrobial delivery system for eugenol.

Different Behavior of Artemisinin and Tetraoxane in the Oxidative Degradation of Phospholipid.

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The reaction of trioxane and tetraoxane endoperoxides with unsaturated phospholipid 1 in the presence of Fe(II) was investigated without oxygen by means of tandem ESI MS analysis. The spectral analyses for the reaction mixtures showed that artemisinin 2 with a trioxane structure gave no peak except the peak of remaining intact phospholipid 1 (m/z 758.9), indicating that any structural change of 1 did not occur. On the other hand, the reaction mixture of 1 with tetraoxanes 3 and 4 afforded a number of new peaks (m/z 620?850) that were presumably assigned to oxidative degradation products originated from the phospholipid 1. Since this reaction was completely inhibited by addition of a phenolic antioxidnat, the process was considered to involve some free radical species. The marked difference in reactivity between the trioxane and the tetraoxanes first discovered must be reflected on the difference in their different anti-malarial mechanisms, and it might contribute to classify a number of anti-malarial endoperoxides based on the phospholipid oxidation.