Society of Cosmetic Chemists Interest Area
Technical Program Abstracts

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SCC 1/BIO 1.1/IOP 1: Biorenewable Polymers

This session developed in conjunction with the Biotechnology and Industrial Oil Products Divisions of AOCS.

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Chairs: R.D. Ashby, USDA, ARS, ERRC, USA; R. Wang, CVC Thermoset Specialties-Emerald Performance Materials, USA; and T. O'Lenick, Society of Cosmetic Chemists/Surfatech Corp., USA

Novel Plant Oil-based Polymers: An Overview. D.J. Kalita[1], I. Tarnavchyk[1], S. Samanta[1], O. Shafranska[1], J. Bahr[2], A. Popadyuk[1], A. Voronov[1], D. Bajwa[3], A. Bezbaruah[4], M. Sibi[5], and B.J. Chisholm*[1,6], [1]Dept. of Coatings & Polymeric Materials, North Dakota State University, USA, [2]Research & Creative Activities, North Dakota State University, USA, [3]Dept. of Mechanical Engineering, North Dakota State University, USA, [4]Dept. of Civil Engineering, North Dakota State University, USA, [5]Dept. of Chemistry & Biochemistry, North Dakota State University, USA, [6]Materials & Nanotechnology Program, North Dakota State University, USA.

A wide variety of homopolymers and copolymers were produced from novel plant oil-based vinyl ether monomers. The monomers were produced by base-catalyzed transesterification of 2-(vinyloxy)ethanol with either a plant oil triglyceride or plant oil-derived methyl esters. By proper choice of the polymerization system, linear polymers were produced that retained the unsaturation derived from the plant oil. By preserving side-chain unsaturation, crosslinked networks were achieved either directly through autoxidation or by post-polymerization modification of the double bonds to other reactive functional groups. Select homopolymers and copolymers were found to have utility for a variety of applications including paints and coatings, shampoos, rubber compounds, and environmental remediation. The results obtained clearly show that this monomer and polymer technology provides new opportunities for the use of plant oils in industrial applications. The general concept has also been used to produce novel monomers and polymers from other renewable resources including cashew nut liquid, terpenes, and lignin.

Sucrose Octaesters as Reactive Diluents for Alkyd Coatings. A. Popadyuk[1], A. Breuer[1], J. Bahr[2], I. Tarnavchyk[3], A. Voronov[3], and B.J. Chisholm*[1,3], [1]Renuvix LLC, USA, [2]Research & Creative Activities, North Dakota State University, USA, [3]Dept. of Coatings & Polymeric Materials, North Dakota State University, USA.

Sucrose octaesters, which are 100% biobased, have been proposed as effective reactive diluents for the production of high-solids alkyd coatings. A series of five different sucrose octaesters (SOEs) derived from soybean oil methyl esters, linseed oil methyl esters, and mixtures of soybean oil and linseed oil methyl esters were synthesized and characterized. The drying-time and cured film properties of the different SOEs produced with the same drier package were determined. In general, increasing the concentration of linseed oil methyl esters used to produce the SOEs decreased drying-time, decreased viscosity, increased hardness, and decreased impact strength. The SOEs were also blended with commercial alkyd resins to produce high-solids alkyd coatings and the drying time and coating properties determined.

Agricultural Waste and Non-traditional Oil in Polyol Synthesis. C.M. Patel, A. Barot, and V. Sinha, V.P. & R.P.T.P. Science College, India.

Biomass including agricultural residues are promising alternatives to petroleum in the production of value-added products. Polyols were synthesized using a two-step process featuring polyhydric alcohols in the presence of various acid catalysts. The steps involved liquefaction of agricultural wastes followed by optimization of process parameters. Polyols were developed using different non-traditional oils to modify the liquefied products. Each polyol was characterized using both chemical and instrumental methods. Results showed that 93% of the solid raw material was converted into polyols in a PEG/Glycerin-based liquefaction system using a solid/solvent ratio of 0.25 in 60-80 minutes at 160°C. The liquefied product showed an I_{OH} of 200 to 400mg KOH/g and a viscosity of 0.93Pas. The developed polyols can be used for development of foams, adhesives, and paints. In the present study, high quality rigid polyurethane foams, commonly used as insulation materials, were developed from bio based polyols. The present work focuses on formulations, applications and property analyses of these polyols.

Shape Memory Polyurethane Elastomers from Vegetable Oils. Z.S. Petrovic and J. Milic, Pittsburg State University, USA.

A shape-memory material "remembers" its original shape and returns to its pre-deformed shape when heated. This material is an alternative to conventional actuators with applications in biomedical and other industries. Novel shape memory polyurethanes were prepared from polyols made by polymerization of hydroxynonanoic acid methyl esters generated by ozonolysis of vegetable oils. Segmented polyurethanes consisted of hard segments from MDI and butane diol and highly crystallizable soft segments of polyhydroxynonanoic acid. The materials behaved as elastomers above melting point of the soft segment and hard plastic below. Melting pointes were tunable between 40 and 60°C. The materials displayed complete recovery of shape and length when heated above the transition point.

Catalytic Copolymerization of Methyl 9,10-epoxystearate and Cyclic Anhydrides. U. Biermann[1], A. Sehlinger[3], M.A.R. Meier[3], and J.O. Metzger[1,2], [1]University of Oldenburg, Germany, [2]abiosus e.V., Germany, [3]Karlsruhe Inst. of Technology, Germany.

Plant oil derived compounds are attractive as raw material for the production of environmentally friendly and in many cases biodegradable consumer products. A great challenge is the production of polymers based on renewable feedstock. We have reported the alternating ring-opening copolymerization of methyl 9,10-epoxystearate with various cyclic acid anhydrides such as phthalic anhydride, succinic anhydride, and maleic anhydride to afford polyesters of narrow molecular weight distributions using a (salen)$Cr^{(III)}Cl$ catalyst in the presence of *n*-Bu_4NCl [1].

In this way, polyesters (M_n =2000-10000g/mol) with low glass transition temperatures were formed. The reaction is characterized by sustainable aspects, for instance, the use of starting materials derived from renewable resources (> 60%), low catalyst loadings, and no added solvent. The pending long chain alkyl groups introduced in the polyesters by the fat derived substrates attribute amorphous properties to the polymers. Various fatty epoxides are easily available and open up the possibility for the synthesis of new highly branched polyesters.

[1] U. Biermann, A. Sehlinger, M. A.R. Meier, J.O. Metzger, *Eur. J. Lipid Sci. Technol.,* DOI: 10.1002/ejlt.201400631

The Development of Polyols and Polyurethane Spray Foam from Canola and Other Prairie Oilseed Crops. J.M. Curtis[1], E. Kharraz[1], X. Kong[1], T.S. Omonov[1], Y.Y. Zhao[1], D. Treleaven[2], M. Kennedy[3], and D. Kennedy[4], [1]Lipid Chemistry Group, Dept. AFNS, University of Alberta, Canada, [2]Meadow Polymers & Consolidated Coatings, Canada, [3]Green Analytics Corp., Canada, [4]Mod Panel Inc., Canada.

The use of lipid feedstocks in chemical manufacturing is well established and these are sustainable alternatives to petrochemicals. Polyols are one such class of compounds, already commercially produced from vegetable oils. Polyols that incorporate lipids range from intact natural polyols, like castor oil, to polyols that retain certain structural elements of natural lipids, such as the triacylglyceride skeleton, and ultimately to complex polyols that little resemble the starting oil. Here we describe our development of such a range of lipid-based polyol structures with possible applications.

As an example, we have developed a polyol from canola oil, now produced at pilot scale with production facility underway. It has low viscosity and high reactivity so is suitable for use in polyurethane (PU) spray foam for building insulation. Renewable, lipid based components like this can improve the overall environmental impact over the life cycle of PU spray foam. We have developed a PU spray foam formulation with comparable properties to current commercial products, e.g. cream time, rising time, curing time, and viscosity, and so can be a direct substitute. Finally, the closed-cell content, density, mechanical properties, water absorption, and aging properties of the partly biobased foam matches existing petrochemical products.

Recent Applications of Biobased Polymer Chemistry Platforms for the Development of Novel Personal Care Ingredients. M.J. Fevola[1], F.C. Sun[1], and S.E. York[2], [1]Johnson & Johnson Consumer Inc., USA, [2]University of Oregon, USA.

Polymeric ingredients are preferred for personal care formulations due to their extraordinary combination of functionality, efficiency, and safety. As manufacturers seek to improve the sustainability of personal care products, they increasingly seek “greener” chemistry platforms for ingredients that will increase the renewable and biodegradable content in their formulations without sacrificing performance. Starch and polyglycerol (PG) are examples of versatile platforms that enable development of a broad range of functional ingredients. This presentation will discuss recent advances in the application of these chemistries for designing new amphiphilic molecules with utility as surfactants, conditioners, and thickeners. A 90% biobased, readily biodegradable polymeric surfactant was developed using alkenylsuccinate modified potato starch. This high foaming, ultra-mild cleansing agent was obtained by precisely controlling the starch molecular weight and degree of hydrophobic substitution. Modification of PG with either hydrophobic or combinations of hydrophilic and hydrophobic quaternary ammonium groups enabled the synthesis of novel compounds useful as skin and hair conditioners due to their substantivity and humectancy. PG-modified hydrophobic esters of methyl glucoside or sorbitan, e.g. dioleates, demonstrated the ability to thicken detersive surfactant systems.

Composite Feed Stocks and Imaging with Fluorescence Lifetime Microcopy. J.W. Woodcock[1], D.M. Fox[1,3], I.A. Sacui[1,2], C.S. Davis[1], and J.W. Gilman[1], [1]National Inst. of Standards & Technology, USA, [2]Georgetown University, USA, [3]American University, USA.

Design of bio-based composites is best accomplished by taking inspiration from nature. Natural composites are inherently multifunctional; often exhibiting attributes such as: strength (toughness), resilience, sensing, self-healing, light weight, degradability, and optical (camouflage, fluorescence). Designing tough composites is both important and difficult, but in natural systems it is accomplished by incorporating both intrinsic and extrinsic toughening mechanisms over multiple length scales. Molecularly flexible biopolymer matrices are often combined with nano- and micro-scale reinforcing particles or fibers. The rich functionality of bio-based components enables exquisite control of the interactions between the two phases, and allows the reinforcing phase to provide the stiffness and the matrix to provide the flexibility. Here we present examples of semi-

crystalline materials that have large potential in conventional composite applications using common thermoset and thermoplastic matrices. We show the use of basic chemistry enables modification of surface chemical potentials to improve composite interactions. In addition, with easily accessible chemistry, metrologies such as fluorescence lifetime microscopy via stimuli responsive molecular probes that were employed to monitor the stress transfer processes at the composite interphase.

Moisture Resistant Coating for Packaging Paper from Silylated Soybean Oil. C. Tambe, D. Graiver*, and R. Narayan, Michigan State University, USA.

A novel approach of silylating internal double bonds of long chain fatty acids is introduced. Hydrosilylation is so far the most popular and commercially employed way for synthesizing organosilicon compounds by grafting silanes on organic compounds by formation of Si-C bonds. Unfortunately, hydrosilylation is most effective with alkenes containing terminal double bonds. In this study, we have introduced a solvent free one step silylation process for the preparation of moisture curable silylated soybean oil. The product was characterized qualitatively by ^{1}H-NMR and ATR-FTIR, while quantified by TGA.

The moisture cure of silylated oil was studied as a function of catalyst concentration, water content, and the temperature of cure. Kraft paper, most widely used in paper packaging, was successfully coated with roll coater. It was followed by a pilot scale up of paper coating process using industrial gravure roll coaters, where more than 50,000 sq. ft. of paper was coated. Coated paper demonstrated up to 50% decrease in Cobb values and a significant decrease in the WVTR values.

SCC 2/S&D 2: Surfactants in Cosmetics

This session developed in conjunction with the Surfactants and Detergents Division.
Chairs: M.S. Vethamuthu, Ashland Specialty Ingredients, USA; and D. Abbeduto, Society of Cosmetic Chemists/Colonial Chemical, Inc., USA

Interaction Between Skin and Surfactants: A Review.
P. Giacomoni, Elan Rose International, USA.

Surfactants are amphiphilic substances used in skin-care products such as cleansers and emulsions. The scientific literature reports experimental observations about the interaction of surfactants with human skin.

When in cleansers or rinse-off products, surfactants provoke the removal of surface lipids with the alteration of the lipid-moisture balance of the skin and excessive dryness as net result. This has depends on the type of surfactant and on the "formula" (e.g. soap *vs* syndet bars). When in emulsions or other leave-on products, surfactants disorganize the lamellar structure of the lipids in the *stratum corneum*. This can facilitate the penetration of allergens such as those contained in cosmetic fragrances.
In vitro, surfactants in the growth medium are toxic to cultured cells and induce cell death by breaking open the cell membrane. This mechanism has been invoked to understand the observation that some surfactants behave as irritants when topically applied. *In vivo*, topically applied surfactants induce xerosis and dissolve specific proteins in the *stratum corneum.*

When in shampoos, surfactants can provoke an undesirable stinging of the eyes during the rinse process. The intensity of the stinging is a function of the size of the micelles, which can be modulated by appropriate ingredients.

Multi Domain Silicone Quaternary Polymers. T. O'Lenick, Siltech LLC, USA.

A series of silicone quaternary polymers have been developed that contain water soluble quaternary groups and water insoluble groups on the same silicone polymer backbone. This development allows for PEG/PPG free silicone polymers that are available in a range of solubility for use in personal care formulations. The ability to change the ratio of these water soluble to water insoluble cationic group within a polymer allows for the synthesis of water soluble, water dispersible and water insoluble polymers. In addition to providing conditioning effects, these products are emulsifiers, and have great aesthetics on the skin. The ability to modify the aesthetics provided by the emulsifier is critical since it has recently been shown that the emulsifier determines the initial feel of an emulsion on the skin not the oil phase.

Reassessing the Foam-boosting Properties of Alkanol Amides. R. Galleguillos and L. Lipp, Lubrizol Co., USA.

The foam boosting properties of alkanolamides and a Glucamate ester, MEGCCO, in various aqueous surfactant systems was investigated using meticulous foam tests. This work was conducted to unambiguously establish the relative foam boosting strength of these molecules on the foam of systems based on the anionic/betaine pair of surfactants. The RAFFA burette method, a Bikerman cylinder variation, and the Foam Double Logistic, FODL, a new method developed by us, were employed to measure foam properties such as flash foam, foam density, foam decay, rates of aeration and lathering as well as the quality of the texture of the foam. The results indicated that the foam boosting effect of alkanolamides was not significant in most of the surfactant systems studied. We found that cocamidopropyl-betaine up to 2wt% was sufficient to improve the foam properties of the anionic surfactant. It was discovered that MEGCCO's foam boosting properties were comparable to the alkanolamides in cases where some degree of foam improvement was observed. These results contradict the widely accepted notion that alkanol amides are strong foam boosters. Furthermore the precision of our foam test methods can be used to design surfactant systems with different foam properties as needed in specific applications.

Surfactants in Personal Care Applications: Advances in Role and Selection of Multifunctional Rheology Modifiers.
M.S. Vethamuthu, E. Di Antonio, S. Ozkan, V. Johnson, and H. Fares, Ashland Specialty Ingredients, USA.

Objective: The aim of this work is to present recent advances in polymeric multi-functional rheology modifiers used in surfactant rich cosmetic products. The presentation would highlight the key functionality, rheological profiles, and parameters used to select polymer mixes to achieve optimum yield stress, shear thinning profile, and good pump ability from typical packaging components used for dispensing.

Method and Results: Steady and dynamic rheological experiments were performed on cosmetic formulations using an AR-G2 stress controlled rheometer. Cone and plate geometry with 60mm radius and cone angle of 2^{o} over a stepped stress ramp from 0.1-100Pa at 2 minutes per step was used to measure the rheological profile at 25 & 45^{o}C. The results will be discussed with respect to zero shear viscosity, yield stress and flow profile for a wide range of polymer structured compositions.

Discussion and Conclusion: The suspension stability of formulations strongly depends on the value of the yield stress and zero shear viscosity. The rheological performance parameters also depend on the composition, namely polymer selected, surfactant types; mix ratio, pH, and co additives. Over structuring formulations will result in unacceptable flow properties and contribute to poor tactile or negative foam sensory ratings during use.

Quantifying Technical Changes in Hair Properties After Treatment. T.A. Evans, TRI Princeton, USA

An ability to technically assess ingredient and product-induced changes in hair is essential to cutting through nebulous consumer language and understanding underlying functionality. For example, it is evident that aesthetically-pleasing lubrication is the source of hair "conditioning" and a plethora of other consumer expressions (softer, smoother, repaired, moisturized, etc.). Further insight and contemplation leads to the conclusion that the sizable daily-use hair care industry simply revolves around laying down and removing of surface deposits – along with the construction of new and attractive marketing messages relating to this technical feat.

Without denigrating the undeniable benefits of such products, certain other hair-related attributes associate with the internal structure (i.e. the cortex) and are therefore unaffected by these treatments. Therefore, we are presented with direction for creating new, novel products that alter hair's properties in ways that have not previously been possible.

This presentation will discuss instrumental assessments of hair's structure and properties to better understand product efficacy and direct future endeavors.

Various Oil Micro-emulsions and Their Possible Benefit for Beauty and Personal Care Products. G.A. Smith, Huntsman Performance Products, USA.

Microemulsions are clear, stable, isotropic liquid mixtures of oil, water and surfactant, frequently in combination with a cosurfactant. The aqueous phase may contain salt(s) and/or other ingredients, and the "oil" may actually be a complex mixture of different hydrocarbons and olefins. In contrast to ordinary emulsions, microemulsions form upon simple mixing of the components and do not require the high shear conditions generally used in the formation of ordinary emulsions.

Microemulsion are having unique properties, namely, ultralow interfacial tension, large interfacial area, thermodynamic stability and the ability to solubilize otherwise immiscible liquids. With our unique system, no salts are necessary and microemulsions have been developed with Essential Oils, Vegetable Oils, Mineral Oil, Octyl Methoxycinnimate, Silicone Oil, and esters.

The micro-emulsions may potentially be used to add these solubilized materials to various beauty & personal care products.

Dealing with Rheological Realities—A Guide to a Clean and Satisfying Life. J.M. Chandler, ACT Solutions Corp., USA.

Consumers do not purchase (and repurchase) such personal cleansing products as shampoos, body washes, facial cleansers, and hand washes merely for their cleaning ability. There is a whole consumer experience that comes into play. A large part of consumer delight, or lack thereof, for a product comes with the flow properties. High measured (Brookfield) viscosity is typically more appealing, offering the allure of richness and high content of good things inside. Unfortunately, many 'thick and rich' formulations exhibit a variety of negative rheological traits.

This presentation will look into how viscosity is built in personal cleansing products, and provide some insight into dealing with formulation issues related our increasingly 'free' consumer society. Getting the rheology right in a personal cleansing product is a big key toward gaining consumer acceptance and excitement. Anything they can buy will clean. So, with the destination assured, it is about the journey.

Natural Fragrance Solubilizers. D. Abbeduto, Colonial Chemical, Inc., USA.

As formulators of personal care products continue to look for alternatives to ethoxylated materials, fragrance solubilization has been an area with few viable alternatives. Now, and increasing number of formulation solutions have become available. A variety of commercially available non-ethoxylated and naturally certified solubilizers will be reviewed with regard to properties, certifications, and usage.

Of particular interest to formulators using these products is the ability to solubilize essential oils using two common techniques: premixed with fragrance and added to fragrance/water mixtures. The efficiency of these solubilizers to produce clear aqueous mixtures in combination with a variety of common essential oils will be examined, as well as how they compare to traditional ethoxylates using the same formulation techniques and clear mixture endpoint.

Performance varies dramatically by essential oil polarity, formulation technique, and solubilzer used. The results will assist formulators to improve their selection of appropriate technologies.

SCC-P: Society of Cosmetic Chemists Poster Session

1. **Axillary Microbiota Variation Across Caucasians, Hispanics, and East Asians.** A. Fan, M. Li, and L. Du-Thumm, Colgate-Palmolive Co., USA.

The microbial community of the human axilla plays a key role in the formation of axillary odor by biotransformation of odorless natural secretions into volatile odorous molecules. It is known that East Asians tend to have lower axillary odor than most other ethnicities, however, how axillary microbiota vary across ethnicities remains largely unknown. We designed the first comprehensive study to investigate the axillary microbiota across three ethnicities. Sixty Caucasians, 60 Hispanics and 49 East Asians were included in the study. The axillary bacteria were collected after two daily deodorant applications followed by sample analysis using a high throughput next-generation DNA sequencing. The study has generated unprecedented depth of data on the axillary microbiota for the three ethnicities under study.

Among the three ethnicity groups, East Asians possessed the highest total bacteria load. Bacteria distribution at the phylum level showed no major difference between Caucasians and Hispanics, while East Asians have higher relative abundance of Proteobacteria and lower relative abundance of Firmicutes than the other two ethnicities. In our analysis, we focused on Corynebacteria and Staphylococci, as the general consensus in the literature is that Corynebacteria lead to pungent, apocrine odor while most Staphylococci species are associated with low “acid” odor with the exception of S. hominis. The relative abundance of Corynebacteria is the highest for Caucasians (3.9% for Caucasians vs. 2.4% for Hispanics and 2.8% for East Asians). Although the majority of the Corynebacteria species are similar among the three ethnicities, unique species were identified for each of the ethnicity groups. Larger differences in Staphylococci composition profiles were observed for East Asians than for Caucasians and Hispanics. For example, East Asians possess much higher levels of odor causing S. hominis, and much lower levels of the odor neutral S. epidermidis than both Caucasians and Hispanics.