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Abstracts

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Preface

Ever since the beginning of its involvement in hair research, TRI/Princeton had been asked frequently by the cosmetic industry to organize conferences on hair science on a regular basis. We hesitated because of our desire not to compete with the Society of Cosmetic Chemists, with which we enjoy a healthy professional association. However, in 2003, the SCC agreed that we could arrange a meeting that would not conflict with either their Scientific Seminars in May or their annual event in December. The result was the First Conference on Applied Hair Science, held June 9–10, 2004. We decided to hold it biennially in even-numbered years, not to conflict with the Hair Science Symposium organized by the German Wool Research Institute (DWI), which is held in Europe in odd-numbered years. Ever since the beginning of my involvement in hair research, nearly two decades ago, there has been a feeling that cosmetic research is 'soft' on science. This view has been changed radically by the industry, with capital investment in R&D and by attracting highly qualified professionals, as evidenced by excellent papers in the SCC's *Journal of Cosmetic Science*. We thought this conference would further affirm to the world the high quality of research conducted in the cosmetic industry today. This has been borne out by the quality of the papers presented in the oral and the poster sessions, and also by the large attendance of professionals from different countries of the globe. Being the first conference on applied hair science, and being uncertain as to the number and the subject matter of the presentations, we could not restrict papers to specific areas of research. This made the organization of the papers in these proceedings difficult. I have tried to arrange them as best I could in a simple order. The first half of the proceedings covers physical and surface chemistry, microscopy, theoretical modeling, and fiber science, and the second half covers photodamage, sun protection, and the chemistry of shampoos and conditioners and other haircare products. I hope these proceedings, now and in the future, will be a good indicator of the quality of research conducted in the cosmetics industry. I also hope that this conference will encourage more innovative research, leading to better products. We thank the SCC for its support and its agreement to publish the papers in a supplement to the *Journal of Cosmetic Science*. We thank our colleagues in the industry for their effort in making this conference a success, a number of cosmetics companies, and *Cosmetics & Toiletries* magazine for its sponsorship of this conference. We thank Eleanor Lehman and her team for organizing the conference and the members of the TRI staff for their help during the conference.

Yash K. Kamath
Conference Chair Research Director
TRI/Princeton

Surfactants, polymers and their nanoparticles for personal care applications

P. Somasundaran, S. Chakraborty, Q. Qiang, P. Deo, J. Wang and R. Zhang
NSF Industry/University Cooperative Research Center for Advanced Studies in Novel Surfactants, Langmuir Center for Colloids and Interface, Columbia University, New York, NY 10027, USA

A 'touch me not' plant folding up rapidly upon being attacked or microbes depositing on teeth or ocean vessels even under hostile conditions are examples in nature that provide inspiration for developing new classes of personal care release or deposition systems. In this paper, development of such systems based on polymer/surfactant colloid chemistry is explored for achieving transport and release of cosmetic and pharmaceutical molecules at desired rates at desired sites. The successful development of products

depends upon understanding and utilizing key interactions among surfactants, polymers and hybrid polymers that are relevant to personal care products. Thus, the absorbed layers or tethers on the particulates can be manipulated for desired dispersion of actives or depositions on substrate under any and all conditions. New hybrid polymers and nanogels have been synthesized for tuning up nanodomains that can extract and deliver at will cosmetics/drugs/toxins by perturbing pH, temperature or ionic strength of the system. Particularly, hydrophobically modified polymers have features of both polymers and surfactants and due to the associative nature of the hydrophobic groups, such polymers can form intramolecular nanodomains for performing carrier functions. Nanogels developed recently include that of polyacrylamide, poly(acrylic acid) and starch nanogels modified for extraction and subsequent slow release of fragrances and overdosed toxic drugs. Binding and release processes were investigated using surface plasmon resonance and fluorescence spectroscopies, powerful techniques for monitoring short term and long term changes.

Structural analysis of human hair fibers under the ultra-high voltage electron microscope

K. Koike, O. Yoshida†, A. Mamada*, T. Watanabe‡, T. Hasegawa‡, A. Kuwae‡ and A. Takaoka‡*
**Tokyo Research Laboratories, Kao Corporation, Sumida, Tokyo, Japan 131-8501,†Tochigi Research Laboratories, Kao Corporation, Haga, Tochigi, Japan 321-3497,‡Research Center for Ultra-high Voltage Electron Microscopy, Osaka University, Suita, Osaka, Japan 656-0871*

Three-dimensional structural analyses of human hair fibers and comparison of the different fibers were tried by using the Ultra-high Voltage Electron Microscope (UHVEM). The analysis condition, sample preparation, and a machine state were adjusted to the suitable condition for tilting observation of from −70° to +70°, at 2° intervals. The tomography of hair fiber was successfully reconstructed from the different angle pictures with IMODE software in a computer. By using UHVEM, the various human hair fibers from Japanese and Caucasians were investigated and discussed about their structures.

Microscopic high-resolution digital volumetric imaging of human hair fibers

J. V. Gruber and R. Kerschman†*
**Arch Personal Care Products, L.P., 70 Tyler Place, South Plainfield, NJ 07080,†Resolution Sciences Corp., 530 Tamal Plaza, Corte Madera, CA 94925, USA*

Methods for examining cationic polymer deposition on hair are well known and polymers such as Polyquaternium-10 have enjoyed a significant commercial impact on shampoos and body washes as unique conditioning materials. It was recently reported that hair can be examined using a new microscopic called Digital Volumetric Imaging or DVI (10). By employing fluorescent dyes, deposition of cationic oligosaccharides onto damaged blond hair fibers was discussed. Because hair auto-fluorescences, the microscope allows for examination of hair fibers directly including viewing of the cuticle, cortex and melanin within the cortex and careful imaging even distinguishes the medulla of the hair fiber. In this paper, examination of six virgin hair types including: (1) Afro-American, (2) Asian, (3) European brown, (4) red, (5) blond and (6) gray was conducted looking for differences that each hair type brings to the visualizing technique. Digital manipulation of the fluorescent data allows for examination of interior hair fiber structures as well as the development of animated movies of three dimensional hair fiber structures.

A reciprocal lattice approach to assessing the luster of hair fibers, based on scattering by periodically deformed cylinders

A. John McKinnon
Canesis Network Ltd, Private Bag 4749, Christchurch, New Zealand

In a recent prize-winning study, Nagase et al. presented an analysis, using geometrical optics, of the perception of luster of hair based on the different directions of light reflection from the front and internal rear

surfaces of the fiber. These two reflections, from cuticle cells inclined to the fiber axis, lead to a specular peak and an associated bright zone, displaced in reflection angle, which is associated with luster perception. This work built upon the experimental observations of Bustard and Smith. Both these papers employed a model of the fiber which may be described as a linear stack of cone frusta, defined by the exposed axial length and angle of inclination to the fiber axis of the cuticle scales. This fiber model is readily amenable to an alternative treatment, in which the model is recognized as a convolution of a cone frustum with a one-dimensional lattice. The scattering properties are then given in reciprocal (scattering) space as the product of the scattering function of a single frustum and that of the one-dimensional lattice. This problem was addressed, in principle, long ago by Bear and Bolduan in work on the scattering of periodically distorted collagen fibrils. The author presents a related theory based on conical shells. It is demonstrated that the scattering from such a model extends over a number of non-equatorial reciprocal lattice planes and is able to reproduce, in a crudely quantitative fashion, several of the features of the experimentally observed scattering. A major benefit of this approach is that it gives a three-dimensional appreciation of light scattering by fibers.

The role of computational fluid dynamics (CFD) in hair science

P. Spicka and E. Grald
Fluent Inc., 10 Cavendish Court, Lebanon, NH 03766

The use of computational fluid dynamics (CFD) as a virtual prototyping tool is widespread in the consumer packaged goods industry. CFD refers to the calculation on a computer of the velocity, pressure, and temperature and chemical species concentrations within a flowing liquid or gas. Because the performance of manufacturing equipment and product designs can be simulated on the computer, the benefit of using CFD is significant time and cost savings when compared to traditional physical testing methods. CFD has been used to design, scale-up and troubleshoot mixing tanks, spray dryers, heat exchangers and other process equipment. Recently, computer models of the capillary wicking process inside fibrous structures have been added to CFD software. These models have been used to gain a better understanding of the absorbent performance of diapers and feminine protection products. The same models can also be used to represent the movement of shampoo, conditioner, colorants and other products through the hair and scalp. In this paper, we provide an introduction to CFD and show some examples of its application to the manufacture of consumer products. We also provide sonic examples to show the potential of CFD for understanding the performance of products applied to the hair and scalp.

Torsional method for evaluating hair damage and performance of hair care ingredients

D. Persaud and Y. K. Kamath
TRI Princeton, P.O. Box 625, Princeton, NJ 08542, USA

In this study, we have developed a single hair fiber torsional pendulum method to determine the role of the cuticle and the cortex on torsional properties with respect to fiber cross-sectional area, fiber rigidity, and energy dissipation at 65% RH and in the wet state. Our results demonstrate that in fine diameter fibers with a high cuticle-to-cortex ratio, the cuticula exert a significant effect on the torsional deformation behavior of hair fibers at both normal humidities and in the wet condition. In addition, our data indicate that energy dissipation is confined to fibers with a high cuticle-to-cortex ratio, and the amount of energy dissipated becomes more pronounced with increasing water content. The torsional properties of hair spray-treated fibers suggest that the deposited hair spray film masks the properties of the base fiber and imparts its own dissipative character to the measurement. Since tensile mechanical properties are often used to make claims about the performance of hair care products, we have compared the results obtained from torsional and tensile measurements on over-processed bleached hair fibers conditioned with Polyquaternium-10 and cetyl trimethylammonium bromide (CETAB) to evaluate which method is more advantageous. Our data demonstrate that torsional measurements can distinguish hair care products

which reinforce the cuticle from those which affect the cortex, while tensile measurements showed no significant differences.

Tensile properties of twisted hair fibers

T. A. Dankovich, Y. K. Kamath and S. Ruetsch
TRI/Princeton, PO Box 625, Princeton, NJ 08542, USA

Hair is routinely twisted during grooming processes, which can cause tangles and lead to breakage of hair fibers. To evaluate the damage caused by twisting hair, the tensile stress–strain properties of single twisted hair fibers were measured by two different experimental procedures: (A) twist at constant length, followed by extension to break (without untwisting); and (B) twist and untwist at constant length, followed by extension to break. In procedure (A), the strength, extension, and initial modulus decreased with increase in twist factor, whereas in procedure (B), the strength and extension did not significantly change from control values, although the initial modulus decreased with increase in twist factor. Furthermore, the degree of recovery from torsional deformation was studied by a variant of procedure (B), where the fiber after untwisting was relaxed for 5 and 10 min, respectively, prior to extension to break. The major conclusion from this study was that at low and moderate twist levels, the tensile mechanical properties of human hair are recoverable.

Influence of antioxidants on the sun protection properties of hair care products

K. Meinert, C. Springob, C. U. Schmidt and T. C. Kripp
Wella AG, Berliner Allee 65, 64274 Darmstadt, Germany

Aim of this study was to determine the influence of commercially available antioxidants on sun protection properties of hair care products. To evaluate changes of human hair L*a*b-color measurements, tensile strength measurements and high-pressure dynamic scanning calorimetry (HPDSC) measurements were carried out. To have a measure for the concentration of the activity of the reactive species, causing hair or color damage, chemiluminescence measurements were carried out. Before the test with the antioxidants experiments were carried out to evaluate effects of varied artificial weathering conditions on physical properties of hair. Here high relative humidity (85%) and low radiant flux (600 W m^{-2}) exhibited the biggest changes in natural hair color but the lowest changes in the in tensile strength and HPDSC measurements. All of the tested antioxidants reduced the chemiluminescence level when used in a pre-sun or after-sun formulation. According to the HPDSC measurements the antioxidants showed a slight increase of the peak temperature and therewith a hint towards a protection effect when used in a pre-sun or after-sun product. In contrast thereto some of the antioxidants reduced the tensile strength of sun care products for hair when added. A slight reduction in the lightening of natural hair color could be observed when antioxidants were present in the sun care formulations. The effect of antioxidants in sun care formulations used on dyed hair was strongly dependent on the shade of hair. The addition of some antioxidants yielded significant improvements of the protection properties of the used sun care product in some measurement methods.

Measurement and prevention of hair photoaging

A. Roddick-Lanzilotta and R. Kelly
Keratec Limited, Keratec Building, Springs Road, Lincoln, Canterbury, Private Bag 4749, Christchurch, New Zealand

Fluorescence spectroscopic measurement of the amino acid tryptophan on the hair fiber surface was extended to include *in situ* fiber irradiation and a novel cyclical wash off, reapplication protocol. When applied to the investigation of a new damage prevention active, it was shown that the active was preferentially degraded in a sacrificial manner and that the underlying fiber surface was maintained in good condition. In addition, tensile strength measurements were performed to assess the mechanical properties of the treated and untreated fibers following UV and sunlight exposure and the results demonstrate the damage prevention effectiveness of the active.

Silicones used in permanent and semi-permanent hair dyes to reduce the fading and color change process of dyed hair occurred by wash-out or UV radiation

A. Schlosser
Wacker Chemical Corporation, 3301 Sutton Road, Adrian, MI 49221-9387, USA

Different kinds of silicones were incorporated directly into permanent and semi-permanent hair dyes. To ensure that the silicone was deposited to the hair fibers Si deposition was measured. Hair treated with a silicone free control or the silicone modified hair dyes was tested for color and lightness change (fading) by washing the treated tresses several times and measuring the color change. In a second experiment, hair treated with permanent hair dye was treated with UV radiation to show if silicones can reduce the color change initiated by UV light. The influence of the silicones to dry combing forces of permanent dyed hair untreated and treated with UV was also investigated. The tests showed that dimethiconol/dimethicone mixtures can reduce the washout of hair colorant clearly and silicone resins like trimethylsiloxysilcate or propylphenylsilsesquioxane are able to decrease the color change occurred by UV radiation in dyed hair.

A new multifunctional, shine-enhancing emollient: PPG-3 benzyl ether myristate

T. Gao, A. Pereira and P. Obukowho
Croda Inc., 300-A Columbus Circle, Edison, NJ 08837, USA

A new emollient ester – Crodamol STS (INCI name: PPG-3 Benzyl Ether Myristate) has been developed and characterized. This special non-volatile emollient is safe to use and provides silicone-like feel and multiple cosmetic functionality. It is a liquid with a viscosity about 100 cps at room temperature. It has a high refractive index – 1.4696, which enhances hair shine, contributes to high gloss in lip products, and reduces whitening effect of fatty alcohols and silica in anti-perspirants/deodorants applications. This emollient has high solubility of UV filters, low skin-spreading factor, and good pigment wetting behavior, which are preferable in sunscreen and make-up formulas to enhance the pigment localization and improve SPF value. In this paper, the chemical structure, physical properties, and various cosmetic applications of the emollient will be discussed. Especially, an objective hair shine (luster) test method (color image analysis) has been established and applied to study the enhancement in hair shine by Crodamol STS in hair spray and hair gel formulations. The objective measurements in hair shine showed good agreement with the results obtained from subjective evaluations. The substantivity of Crodamol STS on hair surface, which was delivered from a rinse-off cream, was also determined by a solvent extraction method.

Effects of arginine on hair damage via oxidative coloring process

E. Oshimura and M. Ino
AminoScience Laboratory, Ajinomoto Co., Inc., Suzuki-cho 1-1, Kawasaki 210-8681, Japan

The purpose of this study was to measure the protective effects of arginine in oxidative coloring or bleaching process. Contact angle measurement, tensile measurement and amino acid analysis were employed. As the first step, it was shown that oxidative coloring or bleaching process decreases hair surface hydrophobicity and tensile strength in wet condition. Next the study has been conducted with coloring agents in which part of the ammonia was replaced with arginine, to find that arginine reduced the oxidative change in contact angle and tensile strength. These results suggest that arginine prevents the undesirable attack by hydrogen peroxide on hair proteins and hair surface lipids. Furthermore, it is also suggested from amino acid analysis that a considerable amount of arginine is deposited on, or in hair fibers from coloring agents.

Protein loss quantification of abraded virgin and abraded bleached hair according to Bradford assay

A. L. S. Silva, A. S. Nunes and J. L. Gesztesi
Natura Inovaçaõ e Tecnologia de Produtos Ltda, Cajamar/SP, 07750-000, Brazil

This study intends to present Bradford assay as an alternative to Lowry test to quantify hair damage during combing or brushing. The protocol involves collecting hair fragments

that are chipped away from hair during these abrasive treatments and quantitatively measuring the amount of protein using an analytical procedure to detect low amounts of proteins. This protein determination method involves the binding of Coomassie Brilliant Blue G-250 to hair protein (keratin). It is quite rapid and sensitive and less prone to interferences as the standard Lowry procedure. The latter is subject to interference from compounds such as lipids, cationic surfactants and EDTA, which are ingredients commonly used in hair care formulations and may lead to a false positive result. These drawbacks should be eliminated when using the so called Bradford method for hair protein quantitation. Our studies showed reproducible results for human hair protein and the developed color was stable for up to one hour. The data also show that virgin hair releases less protein than bleached hair. The amount detected for the former after combing ranges from 0.875 to 1.03 mg g^{-1} of hair and 4.85 to 5.35 mg g^{-1} of hair for the latter.

The application of polymethylene waxes as conditioning agent in hair relaxers

S. Vermeulen, A. Jansen Van Rensburg*, B. van der Merwe*, R. Shalvoy† and S. Willford‡*
**Arch Personal Care Products, USA,†Arch Chemicals, Inc., Cheshire, USA, ‡Arch Personal Care Products, South Plainfield, NJ, USA*

Hair relaxers are harsh chemical treatments that leave the hair dull, dry and limp. There is a constant need for improvement of these products to make them milder and incorporate conditioning properties. Because of the high pH of relaxer or hair straightening systems, most quaternized (conditioning) ingredients are unstable and slowly break down to release ammonia over time, having no conditioning effects by the time the consumers use them. This paper discusses the partial substitution of the fatty alcohols that are traditionally used in relaxer systems with polymethylene wax and the benefits derived from using them. The study included the investigation of synergies among the ingredients, the stabilities of the various systems and comparisons with commercially available systems. The polymethylene wax, used in combination with the mineral oil gel and phosphate salt, coats the hair during the relaxing process, leaving it shiny, soft and conditioned as opposed to the poor condition of the hair relaxed by traditional, commercially available NaOH and LiOH relaxers. An additional benefit of using polymethylene wax in relaxer systems is that the conditioning agents that are normally added to the neutralizing shampoo to repair or mask the damage as a result of the relaxing process can be omitted.

Effects of low-level hydrophobic substitution on conditioning properties of cationic cellulosic polymers in shampoo systems

T. V. Drovetskaya, R. L. Kreeger*, J. L. Amos*, C. B. Davis* and S. Zhou†*
**Amerchol Corporation, A Subsidiary of The Dow Chemical Company, 171 River Road, Piscataway, NJ 08854, †Department of Chemistry, College of Staten Island, and the Graduate Center, City University of New York, 2800 Victory Boulevard, Staten Island, NY 10314, USA*

A new class of cationic conditioning polymers (Polymer SL) has been prepared and evaluated in shampoo formulations. Polymer SL is a family of high viscosity quaternized hydroxyethyl cellulose (HEC) polymers with cationic substitution of trimethyl ammonium and dimethyldodecyl ammonium (Figure 1). SL compositions benefit from hydrophobic character to deliver superior conditioning performance in hair care applications. At the same time, low levels of hydrophobes have been chosen to assure good compatibility with surfactant systems without the complications of associative thickening. The polymers have been evaluated in clear shampoo formulations and two-in-one silicone containing shampoos using objective lab methods and subjective panel evaluation on hair tresses. Commercial conditioning polymers: Polyquaternium-10 (PQ-10) (UCARE Polymer LR-30 M^{TM}3) and Guar Hydroxypropyltrimethylammonium Chloride (Jaguar C-13S$^{®}$4) were used as performance benchmarks. The new hydrophobically-modified cationic polymers demonstrated superior performance in all major categories of conditioning and showed improved silicone deposition from two-in-one systems. Moreover, they retained other good qualities of their PQ-10 structural analogs such as enabling crystal clear

formulations and showing no build-up or volume-down effects on hair. These new polymers were also found to be efficient conditioning agents in different surfactant systems with or without silicones. Supplied by Rhodia.

Enhanced delivery of an anti-dandruff active in a shampoo vehicle

A. Georgalas
New Paradigm Technologies of TRI-K Industries, Inc., 151 Veterans Drive, Northvale, NJ 07647-0128, USA

Formulating a delivery vehicle to enhance activity can potentially give higher activity or allow for adjustment to a lesser percent of active. A study was conducted in which the anti-dandruff active, Octopirox®, INCI Piroctone Olamine [1-Hydroxy-4-methyl-6-(2,4,4-trimethylpentyl)-2(1H)-pyridinone], was incorporated into a simple shampoo base at two levels as well as in the same base with an added amphiphilic surfactant blend (Biobase® SMC) at the lower level. A group of 30 male subjects with moderate to severe dandruff were divided into three groups each of which evaluated one of three products for 4 weeks. Methods of evaluation included gravimetric determination of actual dandruff flakes, fluorescent staining of suspect yeast populations, blind evaluation by trained clinical personnel and panelist self assessment. The study demonstrated that the Octopirox® at 0.2% active delivered in the amphiphile blend was superior to the same level in the simple shampoo base and equivalent in activity to a much higher level (0.5%) in the base only. A proposed mechanism postulates the formation of liposome-like association structures that solubilize and entrap the Octopirox® and deposit is substantively to the scalp for enhanced longer lasting activity.