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Revolutionary Hair Pigmentation Recovery

Award

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How to Overcome the New Challenges in Sun Care

Henkel AG & Co. KGaA

60 Years Sinner Circle:
The Future of Washing and Cleaning

SOFW JOURNAL BEST PAPER AWARD 2020

From Innovative Hair Pigmentation Recovery to Challenges in Sun Protection and to the Sinner Circle: SOFW Journal Reveals this Year's Best Articles Award Winners

Thannhausen, Germany, 31 October 2020. For the first time the SOFW Journal awards authors with the SOFW Journal Best Paper Award 2020.

An independent jury of specialists selected the 3 award winners from a total of 80 articles published during the period of November 2019 until October 2020.

"We want to foster, encourage and preserve the art of writing technical application oriented papers. Simultaneously it is a support in times like these where there are limited opportunities to meet clients face to face, to keep contact and to inform thoroughly of the latest developments. Last but not least we believe that reading technical literature deepens the understanding of the material.", explains Robert Fischer, owner of SOFW Journal.

SOFW Journal congratulates all winners and we are looking forward to many new applications for 2021. Writing technical and applied science-oriented papers may be an effort, yet it is the basis of knowledge and business.

The winner of the first prize is the article:

1 Revolutionary Hair Pigmentation Recovery

Authors: Romain Reynaud, R&D Director; Mathias Fleury, Global Category Manager - Biotech. Actives; Daniel Auriol, Scientific Director Biotechnology & Fractionment; Amandine Scandolera, Ph. D, Head of biological evaluation; Mélanie Pélican, Communications Specialist; Morgane de Tollenaere, Skin Biology Scientist; Emilie Chapuis, Clinical Trial Manager – Givaudan Active Beauty

Abstract: Darkenyl™ is a revolutionary and unique hair repigmenting active ingredient. It has been rationally designed to counteract the biological process of hair greying by combining two synergistic molecules: an optimised plant polyphenol (taxifolin glucoside), triggering the hair follicle stem cells to produce new melanocytes while protecting hair follicles from free radicals (ROS); and a soluble precursor of melanin synthesis (N-acetyl-tyrosine), boosting melanogenesis.

Taxifolin glucoside is a unique stabilised polyphenol shown to reactivate hair bulge stem cells proliferation (+30%) and migration to help repopulating the hair matrix with new melanocytes. Its antioxidant properties enable to reduce free radical damages in hair follicles (-53%) and helps protecting existing melanocytes (+189%). Once the hair matrix has been repopulated with new melanocytes and that both new and existing melanocytes are protected from ROS, Darkenyl™ delivers its melanin synthesis precursor (N-acetyl tyrosine) to reactivate melanogenesis (+364%).

Darkenyl™ therefore features a mode of action inspired from stem cells, and delivers powerful consumer benefits: 3.4 times less white hair in 4 months than a placebo (down to -56% white hair). It is also independent of gender and hair-colour and it ensures a long-lasting efficacy.

As sun protection and sun care has been an ongoing emphasis in modern personal care, it is no surprise that the second prize has been won with this subject. The winner is the paper:

2 How to Overcome the New Challenges in Sun Care

Authors: Myriam Sohn, Stanislaw Krus, Marcel Schnyder, Stephanie Acker, Mechtild Petersen-Thiery, Sascha Pawlowski, Bernd Herzog – BASF Personal Care and Nutrition GmbH, Rheinpromenade 1, 40789 Monheim am Rhein, Germany.

Abstract: Sunscreen producers and UV filter manufacturers are currently facing urgent challenges. On the one hand, the legal situation of two widely used UVB filters Ethylhexyl Methoxycinanamte (EHMC) and Octocrylene (OCR) is unclear due to rising concerns about their safety for humans and the environment; on the other hand, the image of nano particulate UV filters is downgraded in the press and by digital apps questioning their safety profile without scientifically based evidence. Some producers pro-actively remove these UV filters from their new sunscreens' developments which is a real challenge in terms of performance achievement. This paper aims to provide UV filter system alternatives for developing efficient sunscreens without EHMC and OCR. Additionally, it clarifies the safety situation of nano-particulate UV filters and explains their usefulness in sunscreens, providing, however, UV filter system alternatives. Furthermore, this manuscript presents a calculation method to assess the impact of a UV filter combination on the environment and shows that it is possible to develop eco-sustainable sunscreens. Though, each restriction in the choice of UV filters will imply certain compromises.

Last but definitely not least, the third prize comes from the field of home care. The winning topic is not necessarily new, but nevertheless still valid and up-to-date – maybe more than ever.
The winning article of the third prize is:

3 60 Years Sinner Circle: The Future of Washing and Cleaning

Authors: Prof. Dr. Thomas Müller-Kirschbaum, Dipl.-Ing. Arnd Kessler, Dr. Arndt Scheidgen – Henkel AG & Co. KGaA, Henkelstraße 67, 40589 Düsseldorf, Deutschland

Abstract: Since 1959, Sinner's Circle has been describing the influence of chemistry, time, temperature and mechanics on the result of a washing or cleaning process in a qualitative way. With the recent opportunities of digitalization and design of experiment, these variables can now be refined and quantified.

On top of the appliance and the detergent, the digital knowledge of performance as a function of these multiple variables plays an important role. This will enable consumers to tailor and finetune washing and cleaning performance to individual needs and scenarios. These scenarios enable hygienic cleanliness while using resources in an optimal way and ensuring the best level of sustainability.

Revolutionary Hair Pigmentation Recovery

R. Reynaud, M. Fleury, D. Auriol, A. Scandolera, M. Pélican, M. de Tollenaere, E. Chapuis

abstract

Darkenyl™ is a revolutionary and unique hair repigmenting active ingredient. It has been rationally designed to counteract the hair greying biological process, by combining two synergistic molecules: an optimised plant polyphenol (taxifolin glucoside), triggering the hair follicle stem cells to produce new melanocytes, while protecting hair follicles from free radicals (ROS); and a soluble precursor of melanin synthesis (N-acetyl-tyrosine), boosting melanogenesis.

Taxifolin glucoside is a unique stabilised polyphenol shown to reactivate hair bulge stem cells proliferation (+30%) and migration to help repopulating the hair matrix with new melanocytes. Its antioxidant properties enable to reduce free radical damages in hair follicles (-53%) and helps protecting existing melanocytes (+189%). Once the hair matrix has been repopulated with new melanocytes and that both new and existing melanocytes are protected from ROS, Darkenyl™ delivers its melanin synthesis precursor (N-acetyl-tyrosine) to reactivate melanogenesis (+364%).

Darkenyl™ therefore features a mode of action inspired from stem cells, and delivers powerful consumer benefits: 3.4 times less white hair in 4 months than a placebo (down to -56% white hair). It is also gender and hair-colour independent and it ensures a long-lasting efficacy.

Stress, pollution and emotions are making our hair suffer. And whatever the source of problems, people are looking for solutions from the beauty industry, the easiest and most efficient way to get fast results. Consumers perceive the "premature ageing" of hair at two levels, physical and psychological. Actually, over 60% [1] of people in the world are currently bothered by hair color loss, especially people aged between 30 and 44. After this age (45 to 65 years old), 74% [2] of the worldwide population is affected by greying hair. Let's see how Darkenyl™ brings a safe and efficient answer to consumers' haircare need.

If genetics can play a large role in hair whitening, it is now well-known that free radicals are directly inducing the premature greying of hair for both men and women. Most of the existing hair pigmentation solutions are based on hair colorants, artificially repigmenting the hair shaft but not addressing the origins of hair whitening. Two other interacting factors are also part of the progressive loss of hair colour, the diminution of melanocytes number in the hair matrix and the decrease of melanin production by these melanocytes.

A human hair shaft is formed by three different layers: the cuticle (external shell), the cortex (internal part, containing melanin granules, responsible for hair colour), and the medulla (soft core only present in mature white hair). Melanin production in the hair is controlled by melanocytes located in the hair bulb matrix [3]. Their activity is regulated by the normal hair cycle. During the growing phase, the melanin produced by active melanocytes is transferred into cortical keratinocytes resulting in pigmentation of the entire hair shaft. During the catagen phase, the melanocytes will enter in apoptosis, and then disappear during telogen phase [4]. In order to produce a pigmented hair during the new growing phase a new pool of melanocytes will migrate and differentiate from the hair follicle stem cells reservoir to the hair bulb to naturally pigment the new hair [5].

Why do we lose hair colour?

The hair greying is explained by age related functional changes in the stimulation and migration of the stem cells from the bulge, but also by environmental factors. Indeed, the accumulation of reactive oxygen species (ROS) into melanocytes upon ageing will lead to mutations, decrease of antioxidant protection system, inflammation, hair falling and greying [6] through two main actions, decrease of the melanogenesis (lower melanin production by melanocytes) and decrease of the melanocytes number (less melanocytes to produce melanin).

How to act on stem cells to repigment the hair shaft?

Givaudan's experts have designed Darkenyl™ to counteract the hair whitening biological process, by combining two synergistic molecules, the taxifolin glucoside and N-acetyl-tyrosine. The first one is a unique stabilised polyphenol shown to reactivate hair bulge stem cells proliferation (+30%) and migration to help repopulating the hair matrix with new melanocytes. Its antioxidant properties enable to reduce free radical damages in hair follicles (-53%) and helps protecting existing melanocytes

(+189%). Once the hair matrix has been repopulated with new melanocytes and that both new and existing melanocytes are protected from ROS, Darkenyl™ delivers its melanin synthesis precursor (N-acetyl-tyrosine) to reactivate melanogenesis (+364%). In 4 months, it has been demonstrated that Darkenyl™ significantly reduces the proportion and density of white hair (down to -56%), 3.4 times better than a placebo.

Stimulation of hair follicle stem cells and melanogenesis

In vitro tests have been performed to study the stimulation of stem cells. One of them, a transcriptomic analysis, related to genes, has seen the hair follicle stem cells (ORSc) treated with 50µM of taxifolin glucoside (one of the 2 main components of Darkenyl™). The expressions of proliferation genes, hair follicle morphogenesis genes and stem cell maintenance genes were evaluated by RT-qPCR. Results show that taxifolin glucoside significantly increases the expression of these genes. A second test has seen the hair follicle stem cells (ORSc) treated with increasing concentration of taxifolin glucoside. The proliferation of ORSc was evaluated by measuring the incorporation of Bromodeoxyuridine (BrdU) into DNA of proliferating cells. Results show taxifolin glucoside significantly increases the proliferation of the hair follicle stem cells, up to +30% versus positive control (EGF). (**Fig. 1**)

To mimic the natural interaction of keratinocytes and melanocytes in the hair matrix, a co-culture of normal human keratinocytes (NHK) and normal human melanocytes (NHM) were treated with Darkenyl™ at 0.01% or Rapamycin (positive control), or left untreated for 72 hours. The melanin content in the cells supernatant was evaluated by colorimetric assay (405nm). It appears that Darkenyl™ significantly increases the melanogenesis, by +364%. (**Fig. 2**)

Activation of hair follicles defences and pigmentation

The antioxidant and pigmentation related genes activation was conducted *ex vivo* on face lift skin explants from three donors with the average age of 63. A mix of 9 mg of hypoxanthin + 10 units of xantin oxidase have been applied during one hour per day for three days, in order to mimic the oxida-

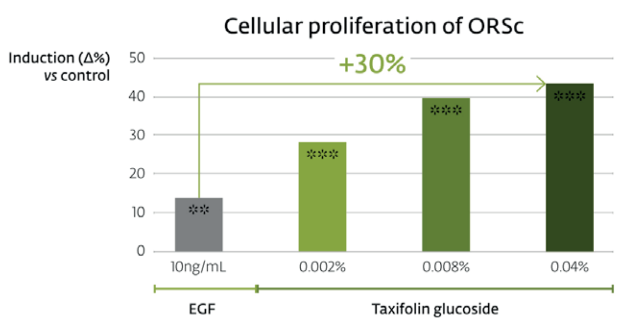

Fig. 1 Cellular proliferation.

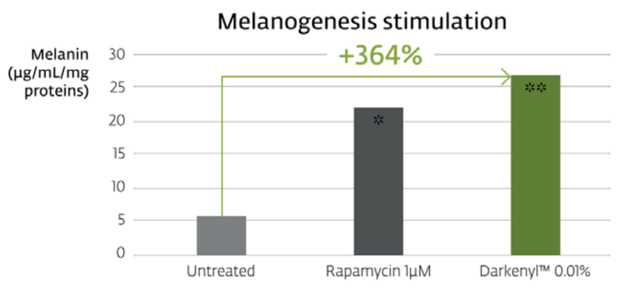

Fig. 2 Melanogenesis stimulation.

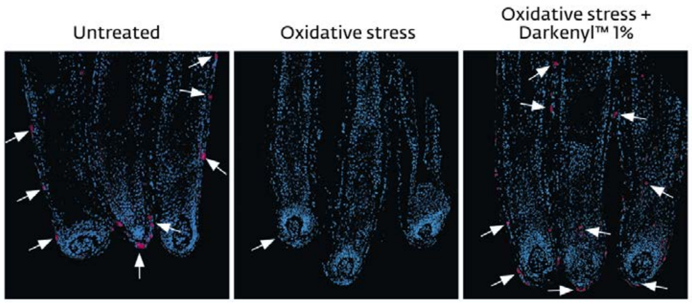

Fig. 3 Melanocytes protection.

tive stress occurring in ageing hair follicle. Then a treatment was done for 48 hours with 1% of Darkenyl™. The expression of genes involved in hair pigmentation, hair renewal and antioxidant defences were measured by RT-qPCR. It appears that under oxidative stress, Darkenyl™ significantly stimulates the expression of these genes.

On the other side, human hair follicles from a female donor (56 years old) were treated with 1% of Darkenyl™ or left untreated. The hair follicles are then exposed to an oxidative stimulus (cumene hydroperoxide – 50µM) for one hour. The ROS accumulation into the hair follicle was evaluated using a green fluorescent probe. Darkenyl™ demonstrates that under oxidative stress, it can significantly decrease by -53% the ROS accumulation into the hair follicle.

Protection of melanocytes during an oxidative stress

Human hair follicles from a female donor (56 years old) were exposed to an oxidative stimulus (cumene hydroperoxide – 50µM) for one hour during an *ex vivo* test. The hair follicles were then treated with 1% of Darkenyl™ or left untreated. The pigmenting cells (melanocytes and melanoblasts) quantification was obtained following NKI/beteb-DAPI double immunostaining. Darkenyl™ significantly protects the melanocytes and melanoblasts into the hair follicle under oxidative stress, by +189%. (**Fig. 3**)

Reaction of pigmentation in white hair

Stimulation of melanin production in greying hair was also tested during an *ex vivo* test. Human hair follicles in anagen phase (growing) from 2 donors (35 and 53 years old) were treated with 1% of Darkenyl™ for 72 hours or left untreated. The melanin content into the hair follicles was evaluated using melanin quantification with Fontana Masson staining and image analysis. Darkenyl™ significantly increases by +15% the production of melanin into the greying hair follicles in 3 days. (**Fig. 4**)

Darkenyl™ reduces white hair in 4 months

The efficacy of Darkenyl™ at 1% was evaluated in a double blind clinical test versus placebo. Forty four Caucasian male volunteers (18 year old and more) with white hair were involved in this evaluation. The panel was split into two groups of twenty two volunteers each, one was testing the placebo and the other one was testing the hair lotion containing 1% of Darkenyl™. The treatment was applied in leave-on by massage on the scalp, once a day for four months. Clinical tests have shown amazing results such as the reduction of the white hair proportion. Pictures of the scalp were taken using a NIKON D7100 in combination with the Canfield Epiflash® system, on the first day of the test and after four months of daily application of the product. The hair parting area was defined according to the white hair localisation. A blind scoring was performed to evaluate the proportion of white hair in the picture versus total number of hair. After four months of treatment, Darkenyl™ significantly decreases the proportion of white hair by an average of -17% versus D0 (from 59% of white hair at D0 down to 49%), 2.1 times better than the placebo. The proportion of white hair is visibly reduced, with a reduction down to -56% for the best respondent (from 90% of white hair at D0 down to only 40% after 4 months). No white roots effect was observed during hair growth. (**Fig. 5**)

To evaluate the efficacy of Darkenyl™ independently from the scalp density, an absolute quantification of the white hair number was also performed. At the beginning of the test, an area of 1 cm^2 was shaved on each panellist's scalp. Two days after shaving, a

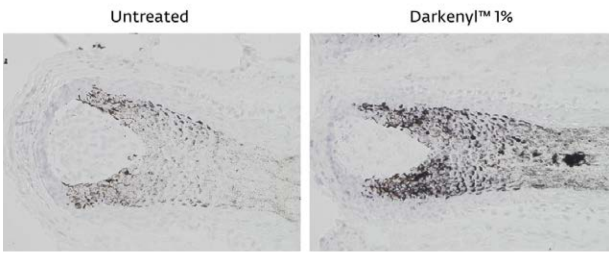

Fig. 4 Melanin production.

Fig. 5 Scalp density.

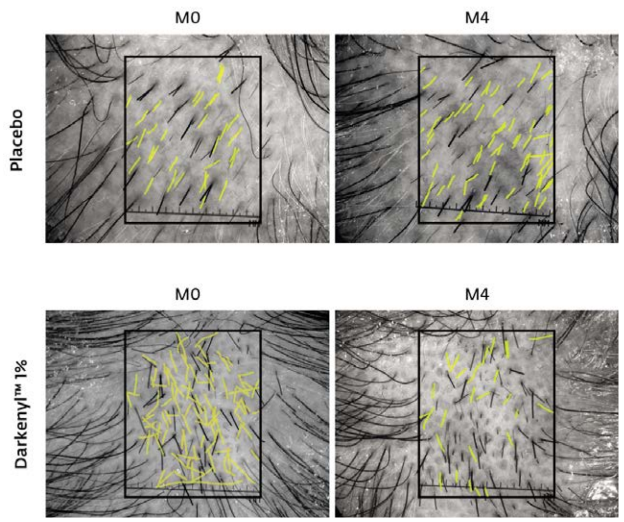

Fig. 6 Hair density.

picture was taken of the area using a NIKON D7100 in combination with the Canfield Epiflash® system. The density of white hair (number/cm^2) was evaluated with a specific Photoshop® tool, on a 0.7 cm^2 test area (1 x 0.7 cm) defined on the image. All white hair whose root was in the analysis zone were counted. After four months of treatment, Darkenyl™ significantly decreases the number of white hair per cm^2 by -6.8, 3.4 times more efficiently than the placebo. The density of white hair is visibly reduced, with up to -55.7 white hair per cm^2 for the best respondent after four months, equivalent to a reduction of -33,420 white hair (the average scalp surface being 600 cm^2). (**Fig. 6**)

Darkenyl™, the perfect innovation to answer a global consumers' need

Most of the existing hair pigmentation solutions are based on hair colorants, artificially repigmenting the hair shaft but not addressing the origins of hair greying – sometimes even generating additional free radicals during their usage. These dyes usually end up with non-natural results (a point of concern for men), and lead to the well-known "white hair roots" effect when hair grow back. Darkenyl™ is rationally inspired from the analysis of biological causes of the hair greying. Its unique mode of action is gender independent and can be used on any hair type or colour. It shows progressive and long-lasting results with no white roots effects. Darkenyl™ is the first active ingredient with clinical evidence versus placebo to reactivate the overall hair pigmentation in a significant way, helping consumers look younger upon time, in a natural way, with their own hair colour. Water soluble and worldwide compliant, this active ingredient is easy to formulate in any haircare formula. By rebooting the native production of hair pigment, Darkenyl™ enables brands and formulators to design new generations of "well-ageing" hair care products while crafting a new sensory beauty gesture answering consumers' expectations number one: "I want to look and feel younger with natural solutions".

To inspire the beauty industry
Our experts of formulation crafted S3D® Colourback, a repigmenting and conditioning serum to beautify and rejuvenate the hair. Featuring Darkenyl™ and ResistHyal®, which is the ultimate hair beauty enhancer (optimised mix of hyaluronic acids), this product quickly penetrates into the scalp and spreads on the hair while activating the repigmentation process and protecting the hair follicles. With its innovative comb, S3D® Colourback enables a precise and effective application, directly on the roots.

An active awarded several time
Since its launch, Darkenyl™ won some impressive awards. It began in 2018, when the active ingredient won the Spotlight On Formulation Award – Haircare Actives Winner during in-cosmetics Asia. 2019 was also a successful year since it won 3 awards, two awards during in-cosmetics global 2019 in Paris, the first one for the Innovation Zone Best ingredient Award 2019 – Bronze and the second one for the Best hair care ingredient awards at the Beauty Industry Awards, but also the 1st prize as Innovation Award 2019 during SEPAWA® Congress.

Leave-in option, the sustainable choice
Reducing the amount of water is also part of our main concern for the sustainability in the beauty industry. This is why Givaudan Active Beauty makes sure that active ingredient such as Darkenyl™ can be used in leave-in formula such as hair colour recovery spray for example.

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How to Overcome the New Challenges in Sun Care

M. Sohn, S. Krus, M. Schnyder, S. Acker, M. Petersen-Thiery, S. Pawlowski, B. Herzog

Sunscreen producers and UV filter manufacturers are currently facing urgent challenges. On the one hand, the legal situation of two widely used UVB filters Ethylhexyl Methoxycinanamte (EHMC) and Octocrylene (OCR) is unclear due to rising concerns on their safety for humans and the environment; on the other hand, the image of nano particulate UV filters is downgraded in the press and by digital apps questioning their safety profile without scientifically based evidence. Some producers pro-actively remove these UV filters from their new sunscreens' developments which is a real challenge in terms of performance achievement. This paper aims to provide UV filter system alternatives for developing efficient sunscreens without EHMC and OCR. Additionally, it clarifies the safety situation of nano-particulate UV filters and explains their usefulness in sunscreens, providing, however, UV filter system alternatives. Furthermore, this manuscript presents a calculation method to assess the impact of a UV filter combination on the environment and shows that it is possible to develop eco-sustainable sunscreens. Though, each restriction in the choice of UV filters will imply certain compromises.

Introduction

Developing new sunscreens has turned out to be highly challenging due to both the unclear fate of some approved UV filters and the hurdles to register new UV filter molecules [1]. From the UV filters under scrutiny, the widely used UVB filters Ethylhexyl Methoxycinnamate (EHMC) and Octocrylene (OCR) are heavily discussed due to rising concerns regarding their safety profile for humans and for the environment. In Europe, legally approved UV filters are additionally assessed by the European Chemical Agency (ECHA) within the Registration, Evaluation, Authorization, and Restriction of Chemicals (REACh) process, like all other industrial chemicals. Also, in the USA, the Food and Drug Administration (FDA) issued a proposed rule to put into effect a final monograph for over-the-counter sunscreen drug products [2]. In its proposal the FDA describes the conditions under which a sunscreen active is Generally Recognized as Safe and Effective (GRASE) and highlights the safety data gaps and additional required data for each already approved UV filter to be included in category I, UV filters with a positive GRASE. In addition to the issues put forward by official authority bodies, sunscreen manufacturers must also consider the perceptions of the end consumers. The uncertainty regarding the legal fate in addition to the reticence of consumers explain the willingness of sunscreen manufacturers to pro-actively remove some widely used UV filters such as EHMC and OCR from their new sunscreen developments. This removal results in a real challenge in terms of performance achievement of sunscreen formulations. Further, in the last years the reputation of nano-particulate UV filters was heavily affected by their downgrade in the press and by consumer apps questioning their safety profile without scientifically-based evidence.

This paper aims at explaining current hurdles in developing new sunscreens and at providing hints how to overcome them. We will discuss the main concerns related to EHMC and OCR and propose solutions to achieve efficient sunscreens without these two UV-absorbers. Furthermore, this paper will discuss the issues regarding UV filters in nano form as well as the impact of UV filters on the environment and propose appropriate solutions for a suitable way forward.

Material and Methods

Formulations for Octocrylene and Ethylhexyl Methoxycinnamate Free Systems

The investigations involved two SPF 30 formulations based either on Diethylamino Hydroxybenzoyl Hexyl Benzoate (DHHB) or on Butyl Methoxydibenzoylmethane (BMDBM) as UVA filter referred to as photostable UVA and partly stabilized UVA, respectively. The two oil-in-water (O/W) sunscreens differed solely in their UV filter combinations (**Tab. 1**) and consisted in an emollient mixture of 3 wt% Dicaprylyl Ether (Cetiol OE),

UV filters	Photostable UVA	Partly stabilized UVA
EHS	5.0%	4.5%
PBSA	–	1.0%
EHT	1.5%	1.5%
TBPT[a]	2.2%	–
BEMT	1.0%	2.5%
DHHB	3.0%	–
BMDBM	–	3.0%

[a] given as active concentration

EHS: Ethylhexyl Salicylate (Neo Heliopan OS) from Symrise, Holzminden, Germany; **PBSA:** Phenylbenzimidazole Sulfonic Acid (Eusolex 232) from Merck, Darmstadt, Germany; **EHT:** Ethylhexyl Triazone (Uvinul® T150); **TBPT:** Tris-Biphenyl Triazone (Tinosorb® A2B); **BEMT:** Bis-ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S), **DHHB:** Diethylamino Hydroxybenzoyl Hexyl Benzoate (Uvinul® A Plus) from BASF SE, Ludwigshafen, Germany; **BMDBM:** Butyl Methoxydibenzoylmethane (Eusolex 9020) from Merck.

Tab. 1 Investigated UV filter combinations for sunscreens without EHMC and OCR.

5 wt% Propylheptyl Caprylate (Cetiol Sensoft), and 10 wt% Dibutyl Adipate (Cetiol B) and an emulsifier mixture of 1% Disodium Cetearyl Sulfosuccinate (Eumulgin Prisma) and 3% Sucrose Polystearate, Hydrogenated Polyisobutene (Emulgade Sucro Plus). In addition to the two sunscreens, the study included a placebo formulation that did not contain any UV filters.

Measurement of Free Radicals

We assessed the number of free radicals generated in the sunscreen probes following UV irradiation according to the method described earlier [3]. Briefly, the number of UV-induced free radicals were measured via electron spin resonance (ESR) spectroscopy (MiniScope MS300, Magnettech GmbH Berlin, Germany) using a spin-probing approach. In this methodology, the spin probe PCA, (2,2,5,5-tetramethyl pyrrolidine N-oxyl, Sigma-Aldrich, Munich, Germany) which is stable over time will react with free radicals produced under UV irradiation to be reduced to the ESR-silent hydroxylamine. UV irradiation of the probes was done with a UV solar simulator 300 W Oriel (Newport). The irradiances as integrated values over the spectral ranges were 23.5 W/m² for the UVB range between 280 and 320 and 180 W/m² for the UVA range between 320 and 400 nm.

Blue Light Transmittance Measurements

To assess the reduction of blue light transmittance with particulate organic UV filters, the transmittance profile of two O/W formulations containing either 5% of Methylene Bis-Benzotriazolyl Tetramethylbutylphenol (MBBT) or 5% Tris-Biphenyl Triazine (TBPT) was measured using a Labsphere UV-2000S device (Labsphere Inc, USA). An amount of 1.2 mg/cm² of the preparation was applied on PMMA plates (SB6 from HelioScreen Labs, FR); three plates were prepared per sample and 5 transmittance measurements were performed per plate after an equilibration period of 30 min at ambient temperature.

Assessment of the EcoSun Pass Value

To assess the impact of a UV filter combination on the environment, we used a calculation method providing the EcoSun Pass value of the investigated UV filter system [1, 4, 5]. To this purpose, each UV filter was ranked according to its environmental hazard profile taking into account all available and reliable environmental fate and ecotoxicological data. The underlying six selected criteria were applied to all UV filters in the same way and allow for an unbiased and transparent assessment resulting in a substance-specific and thus individual hazard profile. The eco-friendliness of a UV filter composition can then be derived based on its individual hazard profiles, taking also into account the efficacy of the composition using the calculated SPF and UVA-PF in relation to the total UV filter concentration. Thus, the EcoSun Pass recognizes both the need for more ecofriendly and highly efficient UV filter compositions. It allows for the selection of the most appropriate candidates due to the combination of both criteria. The higher the EcoSun Pass value, the more environmentally friendly is the tested UV filter combination. Compounds proven to be either endocrine disruptor (according to the WHO definition) for the environment, or confirmed to be PBT, vPvB (according to ECHA guidance R11), or being acute (LC/EC50 < 0.1 mg/L) and/or chronically toxic (NOEC/EC10 < 0.01 mg/L) to aquatic organisms may be a serious threat for the environment and cannot be considered as eco-friendly. UV combinations containing such a UV filter compound will exhibit an EcoSun Pass value of zero. We assessed the EcoSun pass value of five different UV filter combinations with SPF 50 and a ratio UVA-PF/SPF of at least 1/3.

Results

Sunscreens without Octocrylene and Ethylhexyl Methoxycinnamate

OCR and EHMC are worldwide registered UVB filters included in 37% and 44% of the sunscreens launched in 2018, respectively [6]. In addition to their typical usage as UVB filtering molecule, EHMC efficiently solubilizes powdered form UV filters [7] and OCR efficiently photostabilizes instable filters such as BMDBM [8]. Both are currently under the spotlight due to ongoing scientific research, public perception and regulatory measures. Over past years, OCR has been incriminated in a number of adverse effects; it was cited to be a photosensitizer [9], entered the substance evaluation process of the ECHA in 2012 (Community Rolling Action Plan, CoRAP) due to the suspicion of being (very) persistent, (very) bioaccumulative and/or toxic (PBT and/or vPvB), is suspected to show an endocrine

INCI Name	Max %	Status
Camphor Benzalkonium Methosulfate (s57)	6%	Minimally used, < 100 to/a
Homosalate (s12)	10%	On CoRAP list
Benzophenone-3 (s38)	10%	On CoRAP list
Phenylbenzimidazole Sulphonic Acid (s45)	8%	Frequently used and not under evaluation
Terephthalylidene Dicamphor Sulfonic Acid (s71)	10%	Minimally used, < 100 to/a
Butyl Methoxydibenzoylmethane (s66)	5%	On CoRAP list
Benzylidene Camphor Sulfonic Acid (s59)	6%	Minimally used, < 100 to/a
Octocrylene (s32)	10%	On CoRAP list
Polyacrylamidomethyl Benzylidene Camphor (s72)	6%	Minimally used, < 100 to/a
Ethylhexyl Methoxycinnamate (s28)	10%	On CoRAP list
PEG-25 PABA (s03)	10%	Minimally used, < 100 to/a
Isoamyl p-Methoxycinnamate (s27)	10%	On CoRAP list
Ethylhexyl Triazone (s69)	5%	Frequently used and not under evaluation
Drometrizole Trisiloxane (s73)	15%	Minimally used, < 100 to/a
Diethylhexyl Butamido Triazone (s78)	10%	On CoRAP list
4-Methylbenzylidene Camphor (s60)	4%	Minimally used, < 100 to/a
Ethylhexyl Salicylate (s13)	5%	On CoRAP list
Ethylhexyl Dimethyl PABA (s08)	8%	Minimally used, < 100 to/a
Benzophenone-4/-5 (s40)	5%	Frequently used and not under evaluation
Methylene Bis-Benzotriazolyl Tetramethylbutylphenol (s79)	10%	Frequently used and not under evaluation
Disodium Phenyl Dibenzimidazole Tetrasulfonate (s80)	10%	Minimally used, < 100 to/a
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (s81)	10%	Frequently used and not under evaluation
Polysilicone-15 (s74)	10%	Minimally used, < 100 to/a
Titanium Dioxide (nano and non nano) (s75)	25%	On CoRAP list
Diethylamino Hydroxybenzoyl Hexyl Benzoate (s83)	10%	Frequently used and not under evaluation
Tris-Biphenyl Triazine (s84)	10%	Minimally used, < 100 to/a
Zinc Oxide (nano and non nano) (s76)	25%	On CoRAP list
Phenylene Bis-Diphenyltriazine (s86)	5%	Minimally used, < 100 to/a

Tab. 2 Maximum authorized concentration and status of European approved UV filters.

disruptor activity [10], which led to its review at the European level, and is currently subjected to further investigations [11]. Independently, its CLP (classification, labelling and packaging) classification was changed from aquatic chronic 4 to aquatic chronic 1 due to additional ecotoxicologically relevant data. Regarding EHMC, it was added to the CoRAP list of the ECHA in 2014 due to the suspicion of being an endocrine disruptor and/or PBT/vPvB [11]. Furthermore, some studies published the potential impact of certain UV filters including OCR and EHMC on the marine aquatic environment especially on coral reef viability [12–14]. It is worth mentioning that some of the studies provide some shortcomings in the study design and thus may not be considered as being suitable for further regulatory actions. However, some governments took already drastic regulatory actions by banning the sale and use of sunscreen products containing certain sunscreen agents. In fact, Hawaii banned the use of Benzophenone-3 (B-3), and EHMC from January 2019 [15] and Palau the use of B-3, EHMC, OCR, and/or 4-Methylbenzylidene Camphor (4-MBC) from January 2020 [16]. Finally, Brazil government published a draft regulation to control some chemicals to reduce their impact on the environment [17]. This ban proposal includes the use of B-3, EHMC, OCR and 4-MBC. From the UV filters concerned from the different bans, 4-MBC already almost disappeared from the market being used in only 3.6% and 0.9% of sunscreen products launched in 2018 worldwide and in Europe, respectively; the market share of B-3 in Europe is low since other efficient UVA filters are approved in this region [6].

Tab. 2 summarizes the situation of European approved UV filters with their maximum authorized concentration (given in % of the total formulation weight) and their status: i. minimally used (inferior to 100 to/a), ii. placement on CoRAP list for deeper review by ECHA, iii. widely used and not under evaluation.

From 28 UV filters approved in Europe, 12 are not frequently used with an annual tonnage of less than 100; this can be

when the UV filter was newly introduced, or to the opposite because of its old chemistry, or to patent restrictions, to specific exclusivity, or to some other reasons. From the 28 UV filters, 10 are under evaluation by the ECHA, the two main reasons are their suspicion of being endocrine disruptor or PBT and/or vPvB. From the 28 UV filters, only 7 UV filters are frequently used and are not under any ongoing evaluation. Yet, from the latter the frequent use of Benzophenone-4 and Benzophenone-5 is not connected to their use as UV filter in sunscreens; indeed no sunscreen was launched in Europe since the last five years with Benzophenone-5 and only a single product with Benzophenone-4 during the same period of time [18]. The limitation of the use of existing UV filters due to different motivations is not expected to be substituted by the introduction in the market of new UV filtering molecules.
Despite being a cosmetic product in most of the regions, sunscreens are a special product category by themselves. The UV filters are subjected to an official approval process before being listed on a positive list, the annex VI of the cosmetic regulation in Europe [19]. During that process they are subject to an extensive scientific assessment to confirm their safety for human use [20]. Form a global perspective, the last innovative UV absorbing molecules were all developed and first launched within Europe. The generated data were subsequently used for their registration in the other non-EU regions relying on the safety assessment performed for their approval in Europe. An exception remains within the USA where sunscreens are Over-The-Counter drugs regulated by the Food and Drug Administration (FDA), including a much longer lasting approval process. Thus, the last UV filters approved in the USA were Avobenzone (1996) and Zinc Oxide (1998), since then no new UV filter molecule was listed on the sunscreen monograph. Some sunscreen producers used an NDA (new drug application) registration process to market a specific sunscreen containing a UV filter which is not listed on the sunscreen monograph [21].
Phasing out from the use of animal tests for the safety assessment of cosmetic ingredients defined under EC Directive 2003/15 [22] impacts the registration of new UV filters in Europe since a full replacement of the *in vivo* tests is not yet possible using alternative *in vitro* test methods only [1]. This disrupts not only the registration of new UV filters in Europe but also in all other regions following Europe. From March 2009, tests on vertebrates for cosmetic have been prohibited. This applies to ingredients as well as to the sale of finished products containing raw materials tested on vertebrates after that time. The deadline for the marketing ban for finished cosmetic products containing ingredients tested after 2009 on vertebrates was extended to March 2013 for some higher tier tests such as repeated dose toxicity, reproductive toxicity, and toxicokinetic testing. Yet, such animal tests are considered as mandatory under EU REACH regulation for the toxicological assessment of the substance requirements for annual tonnage exceeding 1 to. It is, therefore, difficult or even impossible to comply with both regulatory requirements (i.e. Cosmetics Directive versus REACH) considering a raw material which intended use is exclusively for cosmetic products. It should be kept in mind that Europe still had the biggest market share for sun care in 2017 with 32% [23]. Considering the high development costs and time to market which is roughly 8 to 10 years, the development and registration of a new molecule excluding the European market hence seems rather difficult. Going deeper, Mercosur (South American trade bloc) and ASEAN (Association of Southeast Asian Nations) countries follow Europe with respect to marketing ban of products containing animal (vertebrate) tested ingredients and the registration hurdles of new UV filters in the remaining important markets like China and USA is a further limitation.
The big challenge for near future is, therefore, to develop sunscreens as efficient as they are today, while taking into account that both major UVB filters OCR and EHMC may not be available anymore, without any prospect of the launch of a new UVB filter that might replace these two. From the remaining UVB filters that are registered in most of the countries, excluding the specific situation in the USA, one can identify the efficient 1,3,5-Triazine derivatives as promising alternatives to EHMC and OCR due to their high absorbing efficacy. The performance of salicylate-based UV filters is insufficient to replace EHMC and OCR but they are highly valuable as solubilizers of other crystalline UV filters and are often used in combination.
Tab. 3 summarizes the properties of the alternative UVB filters in Europe. The E(1,1) max value corresponds to the extinction of the studied molecule used in 1% (w/v) solution at an optical thickness of 1 cm at maximum wavelength; it allows a

INCI	E(1,1) max[a]	Handling
Ethylhexyl Triazone (EHT)	1450	Lipophilic powder, to be dissolved
Diethylhexyl Butamido Triazone (DBT)	1450	Lipophilic powder, to be dissolved
Tris Biphenyl Triazine (TBPT)	1040	Water dispersion
Phenylbenzimidazol Sulfonic Acid (PBSA)	930	Water soluble powder, to be neutralized
Titanium Dioxide[b]	243	Lipophilic powder, to be dispersed
Ethylhexyl Salicylate (EHS)	200	Liquid oil
Polysilicone-15	180	Liquid oil
Homosalate (HMS)	165	Liquid oil

[a] closest rounding to a multiple of 5, measurements performed in ethanol for oil soluble, in water for water soluble UV filters;
[b] Titanium Dioxide (and) Aluminum Hydroxide (and) Stearic Acid

Tab. 3 INCI, Efficacy E (1,1) max and handling of alternative UVB filters in Europe.

direct comparison of the performance between the UV filters. The performance of a sunscreen depends not only on UVB but also on UVA filters. There are two commercially available organic UVA filters, DHHB and BMDBM. Since the combination of both is yet limited due to patent-related reasons, the formulator should choose between DHHB and BMDBM. Both are lipophilic molecules solid at ambient temperature that need to be dissolved to perform. SPF and UVA-PF are the main indicators for performance and are evaluated using harmonized ISO methods [24–26]. The loss of performance due to the photoinstability behavior of an individual or a mixture of UV filters are embraced in those methods. Not considered are the other effects due to the photoinstability or the photodegradation products of a UV filter. We compared the efficacy in terms of SPF, UVA-PF, and quantity of generated free radicals of two systems with SPF 30 based either on DHHB or on BMDBM, referred to as photostable UVA and Partly stabilized UVA, respectively (**Tab. 4**). **Fig. 1** displays their photostability profile.

The two systems show the same performance in terms of SPF and UVA-PF the performance indicators generally claimed. However, they differ in their photostability profile. BMDBM is efficiently photostabilized by OCR used at concentrations generally exceeding the concentration of BMDBM. In OCR free systems, the photostabilization of BMDBM relies only on BEMT, another efficient photostabilizer [8]. Since BEMT is used at concentrations much smaller than OCR the photostabilization by BEMT is less efficient than that of OCR and is unsatisfactory for OCR free systems (**Tab. 4**). Although the photoinstability is not reflected in SPF and UVA-PF values, potential adverse effects may exist such as the generation of free radicals. Free radicals may further react with other ingredients of the preparation, which may affect the integrity or efficacy of the formulation or, even worse, react with sensitive skin molecules and produce undesirable reactions [28]. We measured the quantity of free radicals generated following a UV irradiation in the placebo and the two sunscreens. The percentage of free radicals measured in the placebo formulation was close to zero which indicates that the formulation chassis used for the present investigation is not a source of free radical formation. The photostable DHHB-based sunscreen showed a number of free radicals similar to the placebo denoting that the used UV filters did not promote the formation of free radicals. Conversely, the partly photostabilized sunscreen generated ten or more times higher free radicals than the photostable sunscreen, which most likely is attributable to the photoinstability of the UV filter system.

This study disclosed two UV filter system alternatives for developing sunscreens without OCR and EHMC and showed that two preparations with a same SPF and UVA-PF do not show per se the same overall performance. Replacing UVB filter commodities such as EHMC and OCR will with the best of our knowledge lead to an increase in the cost of the whole filter system.

		Placebo	Photo-stable UVA	Partly stabi-lized UVA
UV filters	EHS	–	5.0%	4.5%
	EHT	–	1.5%	1.5%
	PBSA	–	–	1.0%
	TBPT [a]	–	2.2%	–
	BEMT	–	1.0%	2.5%
	DHHB	–	3.0%	–
	BMDBM	–	–	3.0%
Perfor-mance [b]	SPF	–	30	23
	UVA-PF	–	11.7	10.6
% generated free radicals		0.5%	2.7%	28.9%

[a] active amount,
[b] calculated with the BASF sunscreen simulator [27]

Tab. 4 SPF, UVA-PF, and generated free radicals (%) of DHHB or BMDBM based UV filter combinations.

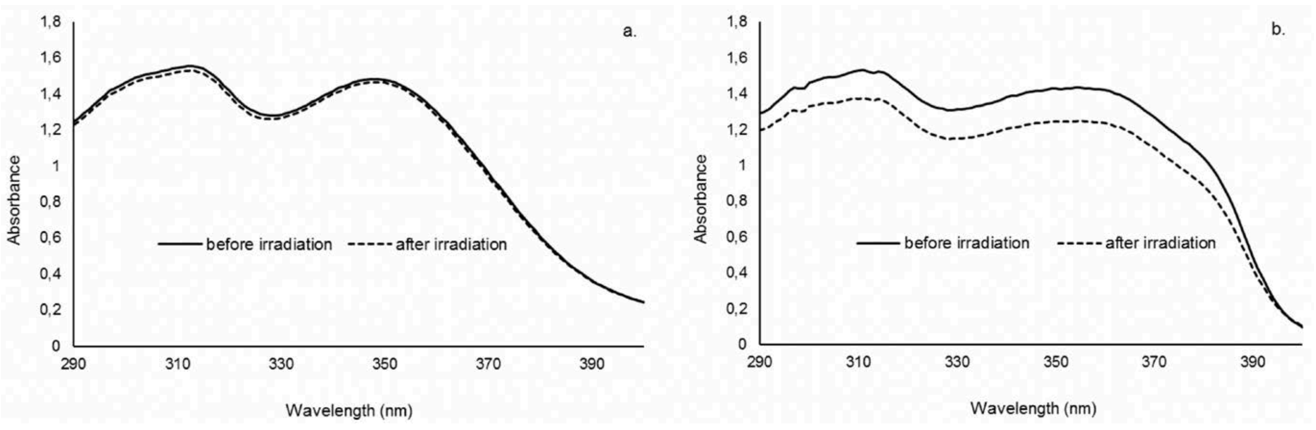

Fig. 1 Photostability profile of a) Photostable UVA and b) Partly stabilized UVA sunscreens; irradiation performed as described in ISO24443:2012.

UV filter	Form	Log Pow	Molecular weight (g/mol)	Median particle size as given in SCCS dossiers
MBBT (nano)	Particulate	12.7 [a]	659/molecule $1.4 \cdot 10^8$/particle	74 nm (FOQELS)
TBPT (nano)	Particulate	10.4 [b]	538/molecule $1.7 \cdot 10^9$/particle	81 nm (FOQELS)
TiO_2 (nano)	Particulate	n.a.	80/molecule $2.3 \cdot 10^8$ – $4.5 \cdot 10^9$/particle	28 to 75 nm (disc centrifuge)
ZnO (nano)	Particulate	n.a.	81/molecule $3.8 \cdot 10^8$ – $2.4 \cdot 10^9$/particle	30 to 55 nm (disc centrifuge)
PBSA	Water soluble	−1.42 [b]	274	< 1 nm
EHMC	Oil soluble	>6 [b]	290	< 1 nm
Polysilicone 15	Oil soluble	n.d.	6000	~ 3 nm

n.a. not applicable; n.d. no data; [a] calculated using the fragment method; [b] measured

Tab. 5 Features of nano and some soluble registered UV filters.

Nano Particulate UV Filters in Sunscreens

The image of UV filters in nano form was damaged due to downgrade in the press and by digital apps for end consumers questioning their safety profile without scientifically based evidences. This section first aims at clarifying the safety situation regarding nano-particulate UV filters and at explaining their usefulness in sunscreens. Though, UV combinations without nano particulate UV filters that might be valuable for spray applications are proposed hereafter.

Safety

The term "nano" is per definition a size descriptor and does not imply any information about human or environmental hazard. EC Regulation No 1223/2009 on cosmetic products defines a nano material as „an insoluble or biopersistant and intentionally manufactured material with one or more external dimensions, or an internal structure, on the scale from 1 to 100 nm" [29]. It seems meaningful to include the insolubility feature of a material to assess the risk since soluble nanoparticles would be dissolved and hence no longer exist in a particulate form. A concern about nano particles is their percutaneous absorption potential. Molecular weight, polarity, melting point, and thermodynamic activity (saturation concentration) of a substance are key features accounting for its skin penetration likelihood [30]. Substances with a melting point below 50°C are more likely to penetrate. Very polar substances with a partition coefficient between octanol and water (log Pow) lower than 1 and very nonpolar substances with a log Pow greater than 4 are unlikely to penetrate the skin. Additionally, according to the 500 Dalton rule, dermal penetration of substances above this molecular mass is significantly decreased [31]. There are currently four nano particulate UV filters registered: the two organic MBBT and TBPT as well as the two inorganic Titanium dioxide (TiO_2) and Zinc Oxide (ZnO) UV filters. All four went through an extensive safety evaluation of their nano form and got a positive SCCS (Scientific Committee on Consumer Safety) opinion. **Tab. 5** provides the features of the nano registered UV filters with the data for some soluble UV filters as comparison purposes. The median particle sizes (D50) were taken from the SCCS dossiers. In the case of MBBT (nano) and TBPT (nano) they were determined with fiber-optic quasi-elastic light scattering (FOQELS). This is a method based on measuring and evaluation of the diffusive particle motion and therefore is only applicable for particles which do not tend to aggregation. When aggregates are formed one would measure the size of those and not the size of the primary particles. It has been shown by electron-microscopic studies that MBBT (nano) an TBPT (nano) do not form aggregates, and thus the size distribution can be measured with this dynamic light scattering technique. With TiO_2 (nano) and ZnO (nano) disc centrifugation was used for the determination of the particle size. Since disc centrifugation is also a method based on particle motion, it is like FOQELS not suitable for particles which may form aggregates, such as TiO_2. Thus, the data given in **Tab. 5** represent most likely not the primary particle size of TiO_2. Assuming spherical geometry, one can estimate the molecular weights of the particles based on their sizes and densities. The densities of MBBT (nano), TBPT (nano), TiO_2 (nano) and ZnO (nano) are 1.12 g/cm³, 1.256 g/cm³, 4.23 g/cm³ and 5.613 g/cm³, respectively.

The log Pow of the organic nano filters MBBT and TBPT is much higher than 4, their water solubility lies in the ng/L range; their molecular weight is over 500 g/mol not to mention the molecular weight of the particles, and the melting point is 196°C and 281°C for MBBT and TBPT, respectively. Taken together these features explain the unlikeliness of nano organic UV filter to penetrate the skin. In respect of their particle size and compared to other soluble UV filters, "Nano means Big". This enlightens why there is no scientific rationale behind the fear of using nano UV filters in sunscreens due to their solely particulate nature.

Efficacy

The organic nano-particulate filters MBBT and TBPT are poorly soluble in oil; for example, the solubility in the common C12-15 Alkyl Benzoate equals 0.29% and 0.029% for MBBT and TBPT, respectively, the solubility of TBPT being one order

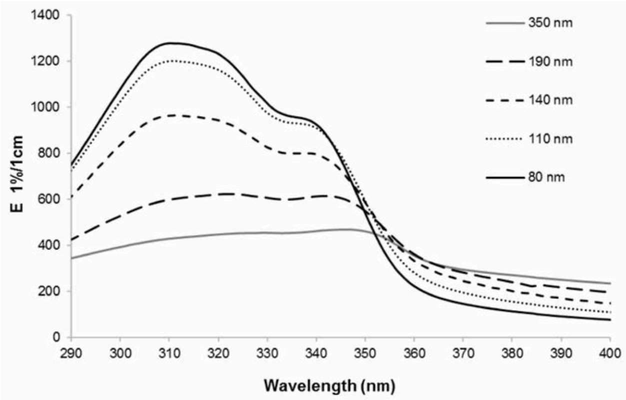

Fig. 2 Specific UV extinction E (1,1) for different particle size of TBPT.

of magnitude lower than that of MBBT. This holds also true for the solubilty in other emollients. For both, the solubility in water is much lower than in oil and lies in the range of some ng/L which makes them ideal candidates for micronization. The reduction of particle size to the nanometer-range is a prerequisite for a satisfactory UV attenuating efficacy of particulate UV-filters. **Fig. 2** illustrates the specific extinction E (1,1) as a function of wavelength for different particle sizes of TBPT. **Fig. 2** clearly shows that with the reduction of particle size a significant increase of the specific extinction of TBPT is achieved. Nano size is a must for all particulate filters to absorb efficiently UV light. However, when size reduction is achieved via milling processes, small particle size means at the same time high energy required by the mill. That means, in practice one has to find a compromise between particle size and energy consumption. It is worthwhile to notice the dependence between the spectrum shape and the particle size; the characteristic absorbance profile of TBPT is connected to its specific particle size.

Furthermore, nano-particulate UV filters show unique benefits compared to soluble UV filters. Due to their particulate nature, a part of the UV light that hits the particle is scattered; the pathlength of the light is increased and the probability that the scattered light is absorbed by another oil soluble UV filter is increased. This boosting of the photoprotection was investigated and described in details by Herzog et al [32]. An additional benefit of the scattering mechanism of the particulate UV filters is the reduction of the transmission in the visible range, especially in the blue waveband, providing an extension of the photoprotection into the visible range as illustrated in **Fig. 3**.

If nevertheless a UV filter combination without nano-particles is required, solutions are presented in **Tab. 6** for SPF 30 to 50+.

Starting from the photostable system based on EHT, DHHB and BEMT as core UV filters, the SPF is adjusted with the addition of either DBT or PBSA. A performance boosting might be obtained using the water soluble UV filter which may, however, become an issue when water resistance is targeted. This is different for the water dispersed nano-particulate UV filters which do not negatively impact the water resistance of a formulation since they are hydrodispersed and not solved in the water phase, the likelihood to be washed off is reduced.

Environmental Impact of Sunscreens

Most of us feel concerned with the climate change and its environmental consequences for our planet, people try to change their behavior to contribute at their level to the protection and saving of our earth. In the cosmetic research, scientists work on sustainable solutions in order to meet both human and environmental safety needs. From the personal care segments, the sun care field is particularly affected by the public discussion regarding the damages UV filters may have on the ecosystem as they are likely to be directly released into the environment. A major recent ecological-related public concern is related to global coral bleaching. Significant contributors to current coral reef bleaching and damaging

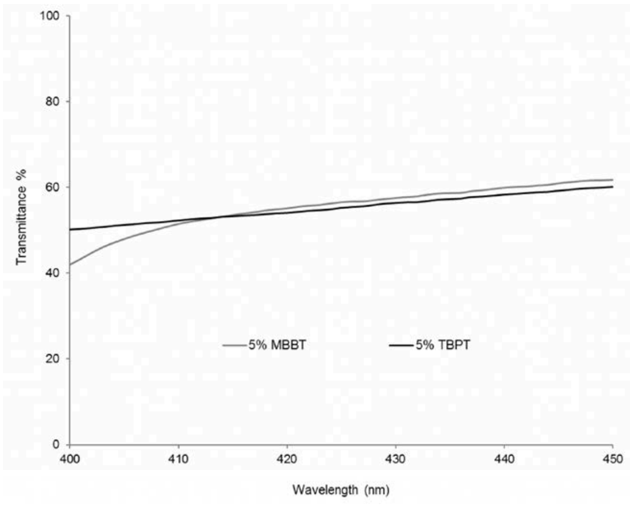

Fig. 3 Reduction of the blue light transmittance by MBBT and TBPT.

UV filters	SPF 30	SPF 50	SPF 50	SPF 50+	SPF 50+
EHS	5.0%	5.0%	–	5.0%	5.0%
EHT	3.0%	3.0%	3.0%	3.0%	3.0%
DBT	–	3.0%	–	4.0%	–
PBSA	–	–	3.5%	–	3.0%
BEMT	2.0%	3.0%	3.0%	3.0%	3.0%
DHHB	4.0%	6.0%	6.0%	6.0%	6.0%
BEMT Aq.[a]	1.0%	1.0%	1.0%	2.5%	2.5%

[a] active amount of BEMT (Tinosorb S Lite Aqua) in the formulation

Tab. 6 UV combinations without nano filters for SPF 30, 50 and 50+ with a ratio UVA-PF/SPF of at least 1/3.

	System 1	System 2	System 3	System 4	System 5
OCR	10.0%	–	–	–	–
EHMC	–	10.0%	–	–	–
EHS	5.0%	5.0%	5.0%	5.0%	–
EHT	–	2.5%	3.0%	2.5%	2.0%
TBPT	3.0%	–	2.0%	3.0%	3.0%
BEMT	2.0%	–	4.0%	1.0%	2.5%
MBBT	–	2.0%	1.5%	2.0%	6.0%
DHHB	–	8.0%	–	4.0%	–
BMDBM	4.0%	–	4.0%	–	–
Total Filter %	24%	27.5%	19.5%	17.5%	13.5%
SPF *in vivo*	53	54	–	53	57
SPF *in silico* [a]	51	50	50	49	49
EcoSun Pass [b]	0	160	195	228	272

[a] calculated with the BASF sunscreen simulator, rounded up to next whole number,
[b] application of the cut-off criterium

Tab. 7 Ecosun Pass value and SPF of five UV filters combinations.

are the increase of the water temperature and ocean acidification through the climate change, marine debris and pollution, physical stress by hurricanes, or fishing practices [33–37]. Independently, some authors investigated the impact of chemicals such as cosmetic UV filters on reef building corals [12–14] initiating the discussion on the impact of sunscreens on corals. Those studies, which at present should be considered as preliminary information only, require in depth assessment and validation (e.g. according to [38]) before they should be taken for any regulatory measures. In addition, the merit of these type of research studies is very often that they are not fit for purpose since study protocols do not follow approved principals of standardized test guidelines and thus important and relevant parameters (i.e. water quality) may have not been measured. For many non-standardised test organisms such as reef building corals, no approved and agreed study protocols exist, which on the other hand triggers the need to develop such test protocols. Meanwhile some governments already took drastic regulatory actions by prohibiting the sale of sunscreens containing some of the worldwide registered UV filters. However, such decisions are problematic since the use of sunscreens has been demonstrated to be highly valuable for human health by helping to prevent skin cancers [39–43], highlighting the importance of scientifically sound hazard and risk assessment.

The market response of some manufacturers to the consumer perception that sunscreens impact the environment is to advertise an improved biodegradability of the formulation, using however a methodology developed for the testing of raw materials and not of finished formulations [44]. Moreover, describing the eco-friendliness of a UV filter combination using biodegradability as single parameter is not sufficient. The assessment of the eco-friendliness of a UV filter system should be a global approach involving all ecological relevant and internationally accepted criteria. To this end, we developed a transparent calculation methodology, termed as EcoSun Pass to investigate the environmental footprint of UV filters and provide a solution to improve the UV filter system to be more eco-compliant. We assessed the impact of five different UV filter combinations with SPF 50 and a ratio UVA-PF/SPF of at least 1/3 on the EcoSun pass value (**Tab. 7**).

All five investigated UV filter combinations show the same efficacy in terms of SPF achieving *in vivo* values of more than 50 which correlate very well with the simulated SPF values. The five systems, however, highly differ in their EcoSun Pass value. The cut-off criterion was applied to System 1 due to chronic toxicity of OCR to aquatic organisms resulting in an EcoSun Pass value of zero; this combination cannot be considered to be eco-compatible. The EcoSun Pass value of the UV combination 2 based on the UVB filter EHMC equals 160. This value is increased in the three systems without EHMC. UV combination 3 based on BMDBM reaches a value of 195, while the value of combination 4 based on DHHB jumps up to 228. Finally, the highest EcoSun Pass value is achieved for the combination 5 which is a mixture of highly efficient and photostable UV filters. Due to the efficiency and photostability of the UV filters the total concentration is much lower than for the other tested combinations. The summation of the excellent environmental hazard score of the UV filters contained in system 5 and the low required concentration explains the high EcoSun Pass value and consequently the eco-friendliness of system 5. This shows that it is possible to develop sunscreens that consider the impact on the environment. However, the cost of an eco-sustainable sunscreen will to the best of our knowledge be higher than the one of a standard sunscreen.

Conclusion

In this contribution we have discussed some urgent challenges sunscreen developers and manufacturers are currently facing, and we have pointed out some possible solutions. However, most of these suggestions imply certain compromises. A compromise may be for instance the acceptance of nano-particulate UV filters when the primary goal is to develop a sunscreen which is safe for the environment and which does contain neither EHMC nor OCR. Another compromise may be to drop the eco-friendliness or water resistance when the target is to be free of nano-particles. Also, each UV filter choice restriction is expected to impact the cost of the product. A new issue is the discussion of microplastics, which affects the whole personal care segment, and also touches sunscreens. Replacing some of the universally used polymers which help ameliorate formulation stability, sensorial properties and water-resistance might become a further new challenge in suncare.

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60 Years Sinner Circle: The Future of Washing and Cleaning

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abstract

Since 1959, Sinner's Circle has been describing the influence of chemistry, time, temperature and mechanics on the result of a washing or cleaning process in a qualitative way. With the recent opportunities of digitalization and design of experiment, these variables can now be refined and quantified.
On top of the appliance and the detergent, the digital knowledge about performance as a function of these multiple variables plays an important role. This will enable consumers to tailor and finetune washing and cleaning performance to individual needs and scenarios. These scenarios enable hygienic cleanliness while using resources in an optimal way and ensuring the best level of sustainability.

Dedication

This paper is dedicated to Dr. Herbert Sinner, a former research chemist at Henkel, recognizing and honoring his contributions for a deeper understanding of the major impact factors in washing and cleaning processes.

1. Historical Background

In 1959, Dr. Herbert Sinner (**Fig. 1**), head of detergents development at Henkel, defined chemistry, mechanical power, temperature and time as the four universal factors which determine the success of a wash cycle [1]. When each of these factors represents a circular sector with a size representing the relative contribution of the particular factor, all four circular sectors have to add up to a full circle, named for its inventor Sinner Circle (**Fig. 2**).
The validity has not changed. But the demands for the several factors have significantly changed. The same is true for their content und understanding. For this reason, the authors extend the development of the Sinner Circle into the future and search to anticipate the future of washing. Four megatrends will have a significant impact: The creation of new business models, new product forms and product designs, new ingredients and cleaning technologies and the requirements of a climate-neutral circular economy. Intensity and dynamics of change are driven by a further growing digitalization and partially just enabled by it.
Herbert Sinner himself developed his circle to describe the new paradigm of washing: washing by hand and in vessels heated by wood or coal fire was substituted by the emerging technology of automated washing machines. For the ecosystem of laundry cleaning, this was a huge paradigm shift, as a new player appeared on the scene: washing machine manu-

Fig. 1 Herbert Sinner [2].

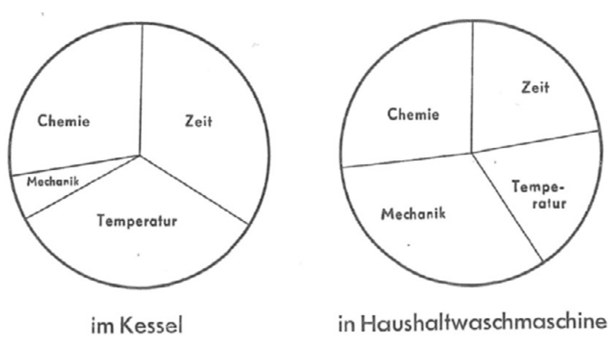

Fig. 2 The original display of the Sinner Circle, comparing the ratios of contributors (chemistry, time, temperature, mechanics) to the washing result in a vessel and in an automated washing machine [1].

facturers, the white goods industry was born. The oldest recycling process of mankind – cleaning clothes to make them wearable again – was based until that time on two main constituents: the person who cleans the laundry mainly by hand with help of mechanical treatment and heating, and the provider of the chemistry that supports this cleaning process. At this very moment of technology change, the manual work of mechanical treatment and the manually steered heating was taken over by a machine. (3) Today we would call it an ecosystem combined with a business model. At Sinner's time, the roles and responsibilities of the participants were very clear: the housewives needed to invest not only into detergents but also into an automatic washing machine.

2. Ecosystem of Laundry Cleaning

And as it was at the time of Herbert Sinner's invention, we are again in the middle of a technological transformation which has at least the revolutionary power for the way how we will do our laundry in the future as it was 60 years ago. The next decades are defined by a transformation towards a climate neutral circular economy. And beside important needs for technological breakthroughs the biggest enabler and influencer is digitalization. By that the ecosystem of laundry cleaning will be defined in a new way and we are witnessing the multiple tremors in all areas of our business.

2.1 New Approaches to Detergent Purchase

At first, the globalization of automated washing has included the huge and fast-growing markets in Asia. And these markets – particularly the Chinese market – are a very special new field for experimentation. For instance, when talking about initiatives by fast growing big players like Haier and Midea in the field of home appliances and manifold start-up companies offering new products and services. But also established global players from our industries – be it in detergents or household appliances – use Asia as a big lab for new approaches. Many of these new attempts might fail, but the new quality is the frequency of challenges to an established system dominated by a consumer who does the washing at home in his or her washing machine and buys regularly one or more detergents for this purpose. How these detergents will arrive at home – by physical or virtual shopping –, could be the topic of an article of its own to speculate about the future roles of manufacturers and established physical and more and more growing virtual retail. The key words are e-commerce, Consumer Relationship Management (CRM), Direct-to-Consumer (D2C), Business-to-Consumer (B2C) and similar.

2.2 New Business Models

The same is true for a second element. While washing at home was the paradigm for the vast majority of households, all partners in today's ecosystem try to find out alternatives to this classical model. For example, detergent manufacturers use the trust in their flagship brands to create laundry services following concepts like dry laundries or – as combination with digitalization and e-commerce logistics – like a laundry service which collects at home, cleans and brings the laundry back home. Or white goods manufacturers think about lease and rent concepts of their machines, as it is already practice for printers and copy machines in most offices.

In this context, we want to start our journey into the future with the typical home washing using a modern washing machine and a modern detergent. The core of business ecosystem was until recent past the "appliance" and "chemistry". Of course, "chemistry" is understood in a much broader sense than only the combination of up to 40 ingredients. As we know we are talking about a very smart optimized synergy of various high-performance materials with an increasing share of biobased and/or biotechnology-based materials.

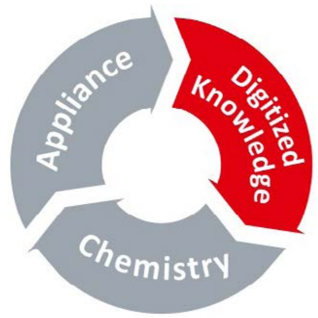

Fig. 3 Digitized knowledge as a complement to appliance and chemistry in the future washing process.

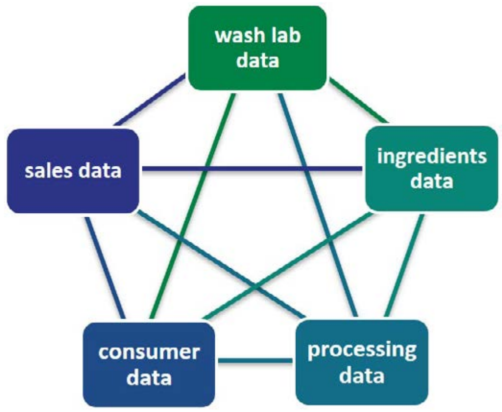

Fig. 4 Various data lakes can be connected to provide the optimal consumer experience.

2.3 Digital Know-how

Now – with the power of digitalization – the core of the ecosystem grows by a third element: the "digital know-how". What do we mean by this? Up to now, the know-how about an optimized washing process was a kind of built-in factor included in the fixed programs of the washing machine and the various detergents with their specific formulations for different washing programs. The digitalization and with its highly sophisticated algorithms allow the combination of the know-how of engineers to run a washing machine and the chemists of developing the best formulations in one overarching software which can – tremendously better than today – orchestrate all the multiple parameters and influencing factors. It is like the "digitalization of the Sinner Circle" or the "Digital Sinner" as we call it (**Fig. 3**).

The digital knowledge goes even beyond the parameters within the appliance. Digitalization allows the combination of data lakes. Wash lab, ingredients, processing, consumer and sales data lakes can be connected in order to provide the optimal washing experience under the best economic and ecological conditions for the consumer. In this article, however, we will focus on the parameters within the appliance (**Fig. 4**).

3. Digitalization of Knowledge through Smart Algorithm

Like industrial processes are reproduced in "digital twins", the digitalization of the Sinner Circle will enable us to create a digital twin of the wash cycle. The idea of a "digital twin" for a washing machine or a "virtual washing machine" is not new. Important research on that topic paved the way for today's digitalization [4, 5]. But at that time, there were just three different equations which described the dependency of one parameter on only four others. It has always been the vision to have all relevant parameters in only one equation with at least 8 or more parameters. And this single algorithm should allow to describe each of them as the function of all the others. By that step, the qualitative relationship formulated by Herbert Sinner will be upgraded into a quantitative parametrization. This will enable fully new opportunities for the prediction and the optimization not only of the four factors of Sinner. Furthermore, additional factors like types and amounts of chemical ingredients, the time those various ingredients or compounds thereof and the dosage at which they are added, as well as different kinds of fabrics need to be integrated into this breakthrough functional relation.

Parametrizing the Sinner factors, it needs to be considered how to make them quantifiable. Parameters for the factor Chemistry are the amount (α), the soiling / stains (σ), the water hardness (θ), furthermore the ingredient split and the dispensing time.

Parameters for the factor Time are the main wash time (t), but also the time at a certain temperature, the soaking time and the after-wash time.

Parameters for the factor Temperature are the peak temperature (τ), but also the temperature profile of the main wash.

Parameters for the factor Mechanics are the laundry load (ω), the fabric type (Λ), the drum speed in the main wash (δ), furthermore changes in the rotation direction and the frequency of active/pause times.

In our approach, we made the Performance (P) a function of the parameters above that are symbolized by letters. Hence, the experiments were performed in the 9-dimensional room given by the following equation:

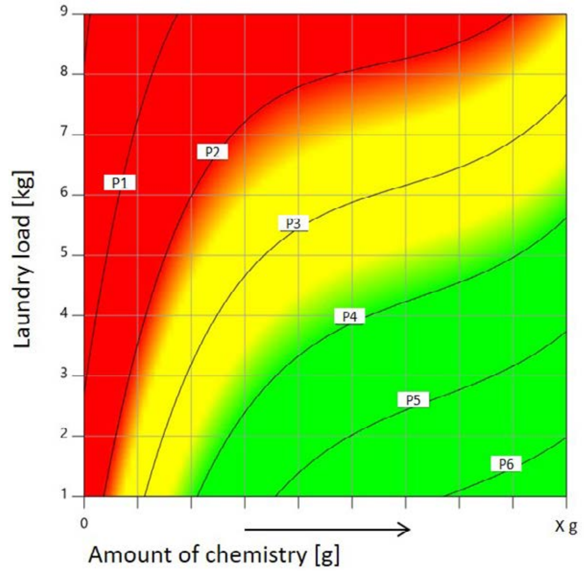

Fig. 5 Performance on an ensemble of 20 stains as a function of the dosage and the load.

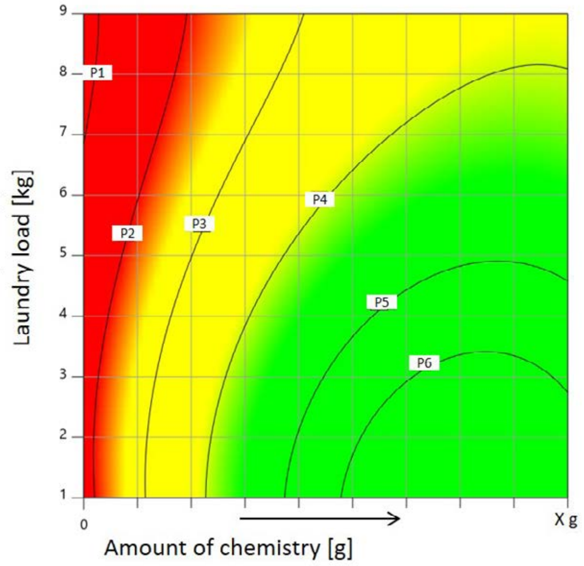

Fig. 6 Performance on an egg stain as a function of the dosage and the load.

$$P = f(\alpha, \sigma, \theta, \omega, \Lambda, \delta, t, \tau)$$

with P = performance; α = amount of chemistry; σ = soiling/stains; θ = water hardness; ω = laundry load; Λ = fabric type; δ = drum speed; t = main wash time; τ = peak temperature.

In **Fig. 5**, the washing performance on an ensemble of 20 stains as a function of the dosage and the load is given. At laundry loads above 6–7 kg, the performance worsens and can be increased by additional detergent dosage.

The washing machine industry has basically developed the major part of programs for the most efficient and most modern machines – the horizontal axis machines – on the base of the former 5-kg wash load machine. In the last decades, consumers have asked for bigger machines and manufacturers have reacted with new machines offering a maximum load of up to 12 kg on a 60 x 60 cm footprint. Dosing schemes provided by the machines – even those for automated dosing of liquids – and the dosing schemes provided by the detergent manufacturers can of course not follow the variation of loads in a continuous way but steer or recommend a dosage for certain clusters [6]. It is quite logical that this is not the optimum which could be achieved when knowing and using the full functional correlation.

The same is true for the quality of textiles. Several programs are designed for specific kinds of fibers. But major challenges occur for mixed fibers. The majority of laundry is based on pure cotton and on cotton-polyester blends. Detergent manufacturers know that a detergent can be optimized on cotton and can be optimized on polyester [7]. Let us imagine that we could read out the weight and type of fiber for every single item the consumer is loading into the washing machine. This technology is not so far away as digitalization, but also increasing electronics technology will allow quite soon an individual RFID or NFC chip printed on a textile and providing this information. Under these circumstances, the Digital Sinner can adapt the dosing of the detergent and – thinking in the direction of dosing several components separately – dose specific ingredients at different amounts.

Another important aspect is the removal of specific stains and/or specific kinds of soil. Some washing machine manufacturers offer advanced programs which are designed to remove specific stains, like a "egg stain program" to remove egg yolk stains. It is very questionable whether consumers use this kind of programs. These programs can only be used if the "stain history" is known, i.e. that the consumer knows the origin and the circumstances how the concerning stain has occurred. Even if this information is given for the specific stain, what about other stains, and are there enough items with tomato stains to start an extra program? And from our consumer research we know that consumers do not know the "stain history" in most cases and expect a washing program and a detergent which can deal with it without this information – at least without the consumer being obliged to provide this information.

The digitalization of the Sinner Circle can make a difference here as well. The parametrization of the washing process includes the functional dependency between the cleaning performance – also for special frequent stains – and all other parameters which can be set accordingly for the machine and the chemistry. In addition, the future home washing machine might have a separate or included stain detection device which identifies the major part of the stains in the various laundry items e.g. in the moment they are put into the washing machine.

In **Fig. 6**, the washing performance on an egg stain as a function of the dosage and the load is given. The performance mainly depends on the detergent dosage, the laundry load plays a minor role.

If appliances or devices can detect specific stains, the washing parameters can be adapted to the problem to be solved.

4. Sustainability and Smart Adaptation of Washing Programs

The Digital Sinner will mark a step change towards sustainability. All dimensions which have already been discussed, describe a new way of washing which "achieves more with less" in general, particularly shorter process, less but right chemistry, more gentle mechanics in the machine. One important factor for optimal performance is of course the right washing temperature. And as we all know, washing at the lowest temperature possible is the major contribution to energy saving and to reduce unneeded CO_2 emission [8, 9].
For this reason, the European detergent industry is advertising a lot for washing at lower temperatures. For example, with the campaign "I prefer 30" [10] as an industry or partially specific consumer advice like the current "Wash Cold" initiative from Henkel. Many consumer associations and institutions for product testing have intensively recommended washing at low temperatures, too. The measurable change in consumer behavior is limited – despite of all this initiatives and advices. Over the last decade we see – if any – only a reduction by very few degrees Celsius.

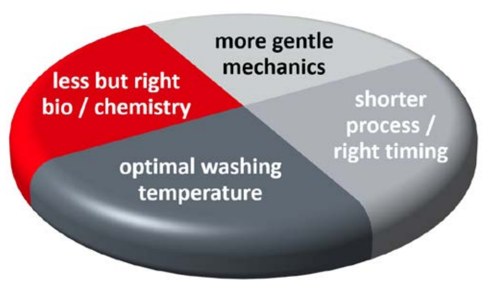

Fig. 7 Opportunities to optimize the parameters of the Sinner Circle.

A significant optimization is possible if the new software decides by itself about the optimal parameters including the right temperature (**Fig. 7**). Consumers will stay in the driver seat as they can select several scenarios for the final result. All the rest will be steered by the smart software of the Digital Sinner. Here are three examples for these kinds of scenarios:

- Quick wash: Dosage, water consumption, temperature and mechanics are adapted to a short washing time in accordance with a pre-selected level of cleaning and with the lowest possible CO_2 footprint [11]
- Ecology: Target is the lowest total environmental footprint in material consumption (dosage) and CO_2 emission in dependency on fibers, filling level, stains, kind of detergent [12]
- Hygiene: Target is the maximum level of hygiene and germ removal by optimizing all other parameters including again the lowest possible environmental footprint [13, 14].

5. Conclusion

The digitalization of the Sinner Circle will allow a more sustainable and more convenient future of the washing process. 60 years after its invention, we are in the middle of the next paradigm shift. The new ecosystem is not any longer built by only the washing machine and the detergent. The "Digitalized Know-how" generates a link between both.
At best both industries will collaborate along the value chain of the newly defined ecosystem in order to shape the future, together.

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