BASF
We create chemistry

Digital simulations of sunscreen performance

ID 579

Sohn, Myriam[1]; Herzog, Bernd[1]

[(1)] BASF Grenzach GmbH, Germany

Introduction

Performance simulations have become the first step of practically any new sunscreen development.
in-silico models are based on the simulation of the transmittance of UV light through an applied layer of sunscreen. The simulation requires quantitative UV absorbance data of all UV-filter substances, their photodegradation characteristics, the photointeraction properties between UV-filters, the oil/water phase repartition synergies and a model to describe the irregularity of the applied film distribution (1,2).
The first model calculations predicted the basic indices of Sun and UVA Protection Factors (SPF & UVA-PF).
Here, we investigated the relevance and usefulness of computational simulations to predict criteria going beyond the SPF and UVA-PF estimations, such as the assessment of the free radical and blue light protection. Furthermore, we described possible use of simulations to predict the impact of the emollients on the performance or to predict the water resistance of sunscreens.

Materials & Methods

SPF and UVA-PF predictions

The simulations are based on the same approach as used for the in vitro SPF and in vitro UVA-PF replacing the measured transmission by the calculated transmission:

$$\text{SPF} = \frac{\sum_{290nm}^{400nm} s_{er}(\lambda)\cdot S(\lambda)}{\sum_{290nm}^{400nm} s_{er}(\lambda)\cdot S(\lambda)\cdot T(\lambda)} \quad \text{Eq(1)}$$

$$\text{UVA-PF} = \frac{\sum_{320nm}^{400nm} s_{ppd}(\lambda)\cdot SUVA(\lambda)}{\sum_{320nm}^{400nm} s_{epd}(\lambda)\cdot SUVA(\lambda)\cdot T(\lambda)} \quad \text{Eq(2)}$$

$s_{er}(\lambda)$ is the erythema action spectrum, $s_{PPD}(\lambda)$ is the persistent pigment darkening action spectrum, $S(\lambda)$ the spectral irradiance, $T(\lambda)$ the calculated transmittance.

Protection against free radicals

Zastrow et al. (3) measured the free radical action spectrum, which revealed that UVB (290-320nm), UVA (320-400nm) and blue light (400-450nm) account for 20%, 63% and 18% of generated free radicals, respectively, underlining the high contribution of UVA irradiation. The free radical protection factor (FR-PF) can be calculated similarly to the SPF and UVA-PF. A radical reduction (%) criterium can be defined:

$$\text{FR-PF} = \frac{\sum_{290nm}^{450nm} s_{r}(\lambda)\cdot S(\lambda)}{\sum_{290nm}^{450nm} s_{r}(\lambda)\cdot S(\lambda)\cdot T(\lambda)} \quad \text{Eq(3)}$$

$$\text{Radical reduction (\%)} = 100 - \frac{100}{FR-} \quad \text{Eq(4)}$$

sr(λ) is the free radical action spectrum

Blue light protection

A factor expressing the protection against blue light can be obtained by considering specifically the wavelength range 400 to 450nm:

$$\text{Blue light protection (\%)} = \left[1 - \frac{\sum_{400}^{450} T(\lambda)}{n}\right]\cdot 100 \quad \text{Eq(5)}$$

n refers to the total number of wavelengths considered between 400-450

Impact of emollients

The calculation of the transmittance is based on experimental absorbance data measured in emollients relevant for sunscreens. The calculated transmittance is then fed into Eq(1) and Eq(2) for simulating SPF and UVA-PF factors of a filter combination in dependence on the emollient (4).

Calculation of water resistance

Here, the computational simulation was used to calculate the SPF using in vitro transmission measurement of a diluted sunscreen solution (5). The sunscreen solution was obtained rinsing off sunscreen-covered substrate plates, subjected or not to a water immersion. The in vitro transmittance is re-calculated for an irregular film structure and fed in Eq(1) to calculate the SPF "no water immersion" and SPF "with water immersion". The water resistance (WR) can then be deduced:

$$\text{Water resistance (\%)} = \frac{\text{in silico SPF no water immersion} - 1}{\text{in silioc SPF with water immersion} - 1}\cdot 100 \quad \text{Eq(6)}$$

Results & Discussion

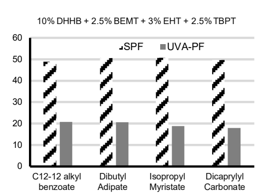
SPF, UVA-PF, free radical, and blue light protection

		Partly stabilized UVA protection	Stable UVA protection	Stable and long UVA protection
Formulation ID		17-214-1-1	17-214-1-2	17-214-1-3
Filter system		5% EHS 2% EHT 2% PBSA 2.5% BEMT 4% BMDBM	5% EHS 4% EHT 2.2% BEMT 4% DHHB	3,5% EHS 0,5% EHT 1,5% TBPT 1% BEMT 4% MBBT 4% DHHB
SPF	In silico	30	30	30
	In vivo (n=5)	-	-	34 ± 4.3
UVA-PF	In silico	10	11	28
	In vitro	-	10	25
Free radicals	In silico radical reduction	79%	87%	95%
	Radicals produced ex vivo (reduction %)	30 ± 8% (70%)	24 ± 4% (76%)	10 ± 5% (90%)
In silico Blue light protection (%)		2%	6%	65%

EHS, Ethylhexyl Salicylate; EHT, Ethylhexyl Triazone; PBSA, Phenylbenzimidazol Sulfonic Acid; BEMT, Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine; BMDBM, Butyl Methoxydibenzoylmethane; DHHB, Diethylamino Hydroxybenzoyl Hexyl Benzoate; MBBT, Methylene Bis-Benzotriazolyl Tetramethylbutylphenol ; TBPT, Tris-Biphenyl Triazine

Simulated values of SPF and UVA-PF were in good agreement with the measured values. The free radical protection increased with an increase of the UVA protection reaching up to 95% reduction of the free radicals theoretically generated using a photostable and long-wave UVA protection. The simulations were in good agreement with the measured ex vivo values.

Impact of emollients on SPF and UVA-PF



The emollient had a negligible effect on SPF and slight effect on UVA-PF attributable to the emollient polarity. Even small, this effect is positive since polar emollients are needed in sunscreens to dissolve solid UV filters.

Calculation of water resistance

	1	2	3
Filter system	3% EHT 3% PBSA 2% BEMT 2% BEMT aq 8% DHHB	3.5% EHT 1.5% PBSA 5% EHS 2.5% BEMT 2% BEMT aq 8% DHHB	3% EHT 5% EHS 3% DBT 3% BEMT 2.5% BEMT aq 6% DHHB
WR in silico	31%	60%	81%

BEMT aq, active of BEMT when used as wáter dispersion (Tinosorb S Lite Aqua)

The WR increased with a decrease of the water-soluble filter; the water dispersed BEMT had no negative effect on the water resistance. This method may be useful to compare a series of formulations.

Conclusions

In-silico models rely on the calculation of the transmission. These data can be used, afterwards, for different purposes as shown here.
Simulations enable an optimization of the UV filter combination before starting laboratory experiments and extensive in vivo performance testing; reducing clinical testing.
Digital methodologies are fast, unlimited in the number of calculations, economical and ethical valuable.

Acknowledgements

Stanislaw Krus
Camille Malburet
Ahim-Galip Caliskan
Jochen Giesinger
Lola Amorós Galicia

References

(1) Herzog, Osterwalder. Simulation of sunscreen performance. Pure Appl Chem 87 (2015) 937–951
(2) Ferrero et al. Efficiency of a continuous height distribution model of sunscreen film geometry to predict a realistic sun protection factor. J Cosmet Sci 54 (2003) 463-481
(3) Zastrow et al. The missing link – light induced (280-1600 nm) free radical formation in human skin. Skin Pharmacol Physiol (2009) 22:31-44
(4) Sohn et al. Effect of emollients on UV filter absorbance and sunscreen efficiency. J Photochem Photobiol B (2020) 205:111818.1–8
(5) Sohn et al. In vitro water resistance testing using SPF simulation based on spectroscopic analysis of rinsed sunscreens. Int J Cosmet Sci (2018) 40:217–225