Ciba® Sunscreen Simulator

Prediction of sun protection factor and UVA parameters

EXPLANATIONS OF METHODS

Calculated SPF

The sun protection factor (SPF) simulation makes use of the formalism first introduce by Sayre in 1979 [1], by which an average of the inverse transmission (1/T) of the respective sunscreen in the spectral range between 290 and 400 nm is calculated, including weighting with a standard sun spectrum, SS(λ), and the erythemal action spectrum, EA(λ):

$$SPF = \frac{\sum_{290}^{400} EA(\lambda) \cdot SS(\lambda)}{\sum_{290}^{400} EA(\lambda) \cdot SS(\lambda) \cdot T(\lambda)}$$

For the simulation the standard sun spectrum was taken from ref. [2], and the erythemal action spectrum from ref. [3].

In order to generate relevant transmission data, the mixed extinction spectrum is calculated according to the amounts and UV spectroscopic performance of the filters and based on an optical pathlength of 20 µm (corresponding approximately to an application amount of 2 mg/cm²). Further, inhomogeneity of the sunscreen film is taken into consideration. A step film model for this purpose had been described by O'Neill in 1984 [4]. The present version of the simulation program makes use of a film profile following an exponential distribution model with two parameters [5]. The parameters were calibrated with standard formulations including the COLIPA P1, P2, and P3 standards. In addition, the calculation takes photoinstabilities of the single filters into account [6] as well as stabilizing and destabilizing effects from inter-molecular interactions [7]. Also the effect of the distribution of the filters in the oil and the water phase of the formulation is taken into consideration for the simulation procedure [8].

Besides the exact calculated value, the program indicates a value rounded in accordance with the international SPF test method [9].

1. R. M. Sayre, P. P. Agin, G. J. LeVee, E. Marlowe. A comparison of *in vivo* and *in vitro* testing of sunscreening formulas, *Photochem. Photobiol*. **29** (1979) 559 - 566

2. B. L. Diffey, J. Robson. A new substrate to measure sunscreen protection factors throughout the ultraviolet spectrum, *J. Soc. Cosmet. Chem.* **40** (1989) 127 – 133

3. A. F. McKinlay, B. L. Diffey: A reference action spectrum for ultraviolet-induced erythema in human skin. *CIE Journal* **6** (1987), 17 – 22

4. J. J. O'Neill, Effect of film irregularities on sunscreen efficacy, *J.Pharm. Sci.* **73**, 888 - 891 (1984)

5. B. Herzog, Prediction of Sun Protection Factors and UV-A Parameters by Calculation of UV Transmissions Through Sunscreen Films of Inhomogenous Surface Structure, Chapter 44 in: Sunscreens: Regulations and Commercial Development (3rd edition), Edited by N. Shaath. Cosmetic Science and Technology Series, Vol 28; Taylor & Francis Group, Boca Raton, FL, 2005, p. 881-900

6. M. Wloka, R. F. M. Lange, H. Flösser-Müller: An in vitro SPF Screening Approach Considering the Photostability of the UV Filters. Proc. Int. Sun Protection Conference, London 2005

7. B. Herzog, S. Mongiat, K. Quass, C. Deshayes, "Prediction of Sun Protection Factors and UVA Parameters by Using a Calibrated Step Film Model", J. Pharm. Sc. 93, 1780 – 1795 (2004)

8. B. Herzog et al., publication in preparation

9. Brown M, SPF Testing in Europe, The International SPF Test Method, Chapter 39 in: Sunscreens: Regulations and Commercial Development (3rd edition), Edited by N. Shaath. Cosmetic Science and Technology Series, Vol 28; Taylor & Francis Group, Boca Raton, FL, 2005, p. 779-806

UVA-PF (PPD)

The most widely used in vivo method for UVA protection assessment is persistent pigment darkening (PPD). PPD is the official method for assessment of the UVA-protection in Japan [10]. Analogue to the erythemal response, which is expressed by the SPF, the UVA-protection factor (UVA-PF) values are determined by the biological endpoint of spontaneous pigmentation after irradiation with an UVA light source. According to the height of the UVA-PF a protection category may be displayed on the package (four categories: -, PA+, PA++, PA+++).

The simulation program determines the UVA-PF in an analogous way as the SPF from calculated transmission data T(λ), now using the spectrum of an UVA lamp, AL(λ), and the PPD action spectrum PA(λ) [8] for calculating the weighted average:

$$UVA - PF = \frac{\sum_{320}^{400} PA(l) \cdot AL(l)}{\sum_{320}^{400} PA(l) \cdot AL(l) \cdot T(l)}$$

As with the SPF calculation, photoinstabilities and effects of the distribution of the filters in the oil and the water phase of the formulation are taken into account.

10. JCIA Measurement Standard for UVA Protection Efficacy, 1995 Japan Cosmetic Industry Association - JCIA, 9-14, Toranomon 2-Chome, Minato-Ku Tokyo, 105

Australian UVA Standard

The Australian Standard 2604 [11] sets out three methods of sample preparation and transmittance measurement in the region of 320 nm to 360 nm for broad-spectrum sunscreen products: The solution method, the thin film method, and the plate method. The program simulates the thin film method, according to which a layer of a braod-spectrum sunscreen product with a thickness of 8 µm shall not transmit more than 10% of radiation at any wavelength from 320 to 360 nm inclusive. Thus, the calculation is based on the transmission spectrum of the respective filter mixture according to a homogeneous film with an optical pathlength of 8 µm.

11. Australian / New Zealand Standard, AS/NZS 2604: 1993

Critical Wavelength

Both, the critical wavelength and the UVA/UVB-ratio are derived from the extinction spectra of sunscreen formulations obtained from in vitro measurements of the transmission on a suitable substrate [12]. Both quantities are reductions of the complete spectral information to one number, characterizing in some way the shape of the spectrum in terms of the amount of UVA-coverage in relation to the amount of UVB-coverage. It is important to note that the algorithm of this reduction is different for the UVA/UVB-ratio and the critical wavelength, and that the information which is left afterwards will not be the same for the both quantities.

The critical wavelength λ_c is defined according to the equation

$$\int_{290}^{l_c} \lg\left[1/T(l)\right] dl = 0.9 \cdot \int_{290}^{400} \lg\left[1/T(l)\right] dl$$

It is the wavelength, at which 90% of the area under the extinction curve between 290 and 400 nm are obtained. The higher the extinction in the UVA, the higher will become λ_c.

Although the Critical Wavelength may be viewed as an alternative to the UVA/UVB-ratio, it has been shown that the dynamic range of λ_c is far more limited. That means that one will achieve saturation of this quantity already at low levels of UVA protection.

12. B. L. Diffey. A method for broad spectrum classification of sunscreens, *Int. J. Cosmet. Sci.* **16** (1994) 47-52

UVA/UVB-ratio

Both, the critical wavelength and the UVA/UVB-ratio are derived from the extinction spectra of sunscreen formulations obtained from in vitro measurements of the transmission on a suitable substrate [12]. Both quantities are reductions of the complete spectral information to one number, characterizing in some way the shape of the spectrum in terms of the amount of UVA-coverage in relation to the amount of UVB-coverage. It is important to note that the algorithm of this reduction is different for the UVA/UVB-ratio and the critical wavelength, and that the information which is left afterwards will not be the same for the both quantities.

The UVA/UVB-ratio is calculated according to the following equation

$$UVA/UVB-ratio = \frac{\int_{320}^{400} \lg\left[1/T(l)\right] dl \Big/ \int_{320}^{400} dl}{\int_{290}^{320} \lg\left[1/T(l)\right] dl \Big/ \int_{290}^{320} dl}$$

Thus it is the ratio of the average extinctions in the UVA- and the UVB-range, and therefore it is a quantity describing the extinction in the UVA range relative to that in the UVB range.

12. B. L. Diffey. A method for broad spectrum classification of sunscreens, *Int. J. Cosmet. Sci.* **16** (1994) 47-52

BOOTS Star Rating System

The Boots star rating system is based on the UVA/UVB-ratio [13]:

UVA/UVB-ratio	0 - 0.2	0.21 - 0.4	0.41 - 0.6	0.61 - 0.8	0.81 - 0.9	> 0.91
Stars	-	1	2	3	4	5
Category	No claim	Minimum	Moderate	Good	Superior	Ultra

13. The Revised Guidelines to the Practical Measurement of UVA:UVB Ratios According to The Boots Star Rating System, The Boots CO PLC, 2004

UVA- Balance and UVA-PF (DIN)

An in vitro UVA-PF may be determined making use of the labeled SPF and the in vitro SPF. In DIN 67502 [14] it is described how this in vitro UVA-PF can be obtained by an in vitro measurement of the transmissions in the spectral range between 290 an 400 nm when the in vivo SPF is known. In a first step the transmission spectrum T(λ) obtained from the in vitro measurement is adjusted by applying a parameter c as exponent to the transmissions, such that the in vitro SPF equals the in vivo SPF (SS(λ): standard sun spectrum, EA(λ): erythemal action spectrum):

$$SPF(vivo) = SPF(vitro) = \frac{\sum_{290}^{400} EA(\lambda)\cdot SS(\lambda)}{\sum_{290}^{400} EA(\lambda)\cdot SS(\lambda)\cdot T(\lambda)^{c}}$$

In a second step the transformed transmsission spectrum $T(\lambda)^c$ is used to calculate the in vitro UVA-PF using the spectrum of the UVA-lamp and the PPD action spectrum described by Chardon [15] according to:

$$UVA-PF(vitro) = \frac{\sum_{320}^{400} PA(\lambda)\cdot AL(\lambda)}{\sum_{320}^{400} PA(\lambda)\cdot AL(\lambda)\cdot T(\lambda)^{c}}$$

where PA(λ) = PPD action spectrum and AL(λ) is the spectrum of the UVA-lamp. A good correlation of the in vitro UVA-PF with the UVA-PF obtained from in vivo PPD measurements has been reported [16]. From the in vitro UVA-PF and the labeled SPF the UVA-balance is derived:

$$UVA-Balance = \frac{UVA-PF(vitro)-1}{SPF(vivo)-1}\cdot 100$$

The simulation program offers two possibilities to obtain the UVA-balance: In the first, the calculated SPF is used in order to adjust the non-irradiated “calculated in vitro” transmission spectrum. In addition, a labeled SPF can be put in, and the program again adjusts the “calculated in vitro” transmission spectrum in order to obtain the in vitro UVA-PF and the UVA-balance. The “calculated in vitro” transmission spectrum for the UVA-balance is obtained in accordance to the description in DIN 67502 by simulation of the extinctions obtained on PMMA substrates using a polynomial expansion of the corresponding extinctions on a homogeneous film [17].

14. DIN 67502: Charakterisierung der UVA-Schutzwirkung von dermalen Sonnenschutzmitteln durch Transmissionsmessungen unter Berücksichtigung des Lichtschutzfaktors, ICS 71.100.70, Deutsches Institut für Normung, Berlin 2005

15. A. Chardon, D. Moyal, and C. Hourseau. Persistent pigment-darkening response as a method for evaluation of ultraviolet A protection assays. *Sunscreens: Development, Evaluation, and Regulatory Aspects*, ed. Lowe, N.J., Shaath, N.A., Pathak, M.A., 559-582, 2nd Ed., Marcel Dekker, New York (1997)

16. V. Wendel, E. Klette, H. Gers-Barlag. A new in vitro test method to assess the UVA protection performance of sun care products, *SÖFW Journal* 127 (2001) 12 – 15

17. “Sandblasted PMMA”, Schönberg GmbH & Co KG, Flagentwiet 29/31, 22457 Hamburg, Germany