The Use of Near-Infrared Spectroscopy and Chemometrics for Determining the Shelf-Life of Products

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In this work a procedure for determining the shelf-life of products by merging near-infrared (NIR) spectroscopy, multivariate techniques of data analysis, and kinetic theory is presented. This procedure allows information from several sources (sensory, physical chemical, and instrumental) to be merged via the multivariate accelerated shelf-life test (MASLT) algorithm. The MASLT is a multivariate approach that relies on soft modeling via an unfolding principal component analysis (u-PCA) and hard modeling, through the conventional kinetic theory, for determining the final shelf-life of products. The procedure was successfully applied to a consumer goods product (a body lotion), whose shelf-life was determined to be 3 years and 9 months, in accordance with results previously obtained using conventional analytical techniques and univariate methods of data analysis.

Index Headings: Stability; Fragrance; Principal component analysis; PCA; Kinetics; Emulsion; Multivariate; Multivariate accelerated shelf-life test; MASLT.

INTRODUCTION

The development of new products demands a considerable amount of human and financial resources. Indeed, it might take months or even years for a new product to be launched onto the market, depending on the degree of complexity of the technology being developed.

One of the most important activities within the development of new consumer goods is the determination of its shelf-life, i.e., the period of time in which it is capable of keeping its quality characteristics within acceptable levels. Despite the determination of the shelf-life of products constituting one of the most time- and resource-consuming activities during the development of novel consumer goods, this mandatory stage must be carefully conducted not only to cope with specific regulatory demands but, most importantly, to deliver the expected benefits to the consumers.

Skin care products, such as body lotions, play an important role within the cosmetics industry. Its primary function is to condition the skin, delivering the right level of moisture and/or preventing the skin from losing water via the use of emollients.[1] However, even a product that is technically capable of providing skin moisturizing will not succeed in the market if it does not deliver important secondary benefits to the consumer, such as superior fragrance performance, suitable viscosity, etc. Fragrance and viscosity are indeed the most valued attributes by the consumers in a body lotion. While the fragrance has to keep its character and intensity during and after use, the emulsion has to be stable during the whole shelf-life of the product.

Fragrance character and intensity, as well as color and emulsion viscosity, are commonly evaluated by sensory panels using a fresh product as reference. However, since the results of these assessments are subjected to considerable fluctuations, the sensory information is seldom used for performing kinetic calculations. Nevertheless, since human sensitivity is usually significantly different from the electronic signals that modern instrumentation supplies, the cut-off criteria are still given by sensory evaluation. The quantitative calculations for determining the shelf-life of body lotions are performed on the results of physical chemical analysis, such as water content, viscosity, droplet size, and gas chromatography. However, these chemical determinations are usually time and resource consuming.

The determination of the shelf-life of a consumer good product relies on the kinetic theory, by which the degradation of a given property of the product is given by:[2–4]

$$v = \frac{dP}{dt} = \pm k_T P^n \tag{1}$$

where v is the velocity of degradation, P is any relevant property that defines the quality of the product, n corresponds to the reaction pseudo-order, and k_T is the rate constant at a given temperature T.

Experience shows that most properties of consumer goods follow pseudo-zero-, pseudo-first-, or pseudo-second-order kinetics (i.e., $n = 0$, 1, or 2). Therefore, both the reaction order and the rate constants are determined by fitting straight lines to the integrated solutions of Eq. 1 (Table I).[2–4]

Conducting a complete shelf-life test on long-lasting products can still demand massive amounts of resources and, most importantly, lead to delays in releasing novel products. Therefore, for speeding up the development of new consumer goods, scientists usually rely on accelerated shelf-life tests (ASLT), which consist of submitting the product to relatively severe conditions of storage. Because k_T is temperature dependent since most degradation reactions are Arrhenius-like (Eq. 2), the harsher conditions to which products are submitted usually refer to some relatively higher temperature of storage.[2–5]

$$k_T = k_0 e^{-E_a/RT} \tag{2}$$

in which k_0 is the pre-exponential or frequency term, E_a is the activation energy, R is the gas constant, and the temperature T is expressed in Kelvin.

The activation energy is the minimum amount of energy necessary for a reaction or degradation process to occur and is determined in practice as the slope of the $1/T$ vs. $\ln(k_T)$ chart. Additionally, the activation energy is an extremely relevant parameter in shelf-life studies since it determines how sensitive a given property is to temperature change.[2–5]

TABLE I. Integrated solutions of typical kinetic pseudo-orders related to the most common degradation reactions of products.

Reaction pseudo-orders	Rate laws	Integrated solutions
Zero	$\dfrac{dP}{dt} = k_T$	$P - P_0 = k_T t$
First	$\dfrac{dP}{dt} = k_T P$	$\ln\left(\dfrac{P}{P_0}\right) = k_T t$
Second	$\dfrac{dP}{dt} = k_T P^2$	$\dfrac{1}{P} - \dfrac{1}{P_0} = k_T$

For estimating the shelf-life of products stored at room temperatures it is necessary to project the results of the accelerated tests onto those of the actual market conditions, which is achieved through the acceleration factor:[2–5]

$$\alpha_{T+\delta T, T} = \frac{v_{T+\delta T}}{v_T} \qquad (3)$$

in which $\alpha_{T+\delta T, T}$ is the acceleration factor and $v_{T+\delta T}$ and v_T are, respectively, the degradation velocities of a given property for the accelerated and for the actual market condition. When the degradation process of products stored at different temperatures follows the same reaction order, Eq. 3 simplifies to

$$\alpha_{T+\delta T, T} = \frac{k_{T+\delta T}}{k_T} \qquad (4)$$

There are well-established protocols reported in the literature for conducting practical accelerated shelf-life studies when formal chemical, physical, or sensorial properties are studied.[2–5] These procedures are mainly composed of three steps: (1) specification of the properties to monitor and their cut-off criteria, as well as the storage conditions to which the product will be submitted (the planning); (2) the storage and data acquisition stage (the execution); and (3) the data analysis, according to kinetic models, for determining the rate constants and the acceleration factors. These steps lead to the estimation of the shelf-life of the product.

Nevertheless, there is currently no shelf-life theory capable of directly linking instrumental data of a multivariate nature and the classical kinetic models. For such studies to be successful, it is mandatory for the instrumental techniques to be able to detect changes in the relevant properties of products with the desired sensitivity.

Near-infrared (NIR) spectroscopy is a cheap, fast, and reliable source of quantitative chemical information for determining the valid date of cosmetic products. The difficulty of directly using NIR for shelf-life analysis lies in its multivariate character. Chen, Hufman, and Park[6] pioneered the use of NIR spectroscopy for studying product deterioration by determining that the spectral changes were strongly correlated with the degradation of mioglobine in chicken meat. The same strategy was followed by Nielsen et al.[7] for estimating the freshness of meat. More recently, Sinelli and colleagues developed studies using NIR spectroscopy for studying the degradation of cheese.[8,9] Nevertheless, these works are limited in the sense that they relied on information provided by NIR spectroscopy solely for indirectly studying the degradation mechanisms of products but did not provide the mathematical basis for directly using the instrumental

signals for applying the kinetic theory in order to quantitatively determine the actual shelf-life of products.

Nevertheless, chemometrics offers a robust set of tools that take advantage of the multivariate nature of NIR spectroscopy for providing quantitative information to be used for performing kinetic calculations, as well as allowing interpretations to be performed.

THE MULTIVARIATE ACCELERATED SHELF-LIFE TEST

The multivariate accelerated shelf-life test (MASLT) was previously developed by the authors[10] for handling shelf-life studies possessing several properties, especially sensorial attributes. It is a functionalized unfolding principal components analysis (u-PCA)[11,12] in which the scores are used as properties in the shelf-life calculations while the loadings are used for interpreting which variables have had a significant influence on product degradation. When NIR spectroscopy is applied, the variables are wavenumbers that can be associated with chemical and/or physical phenomena occurring in the product as a function of time.

The main assumption of the MASLT is that the reactions responsible for the changes in the product's characteristics are the main source of variation in the data set and, therefore, the PCA should be driven by time-related phenomena. Moreover, as the PCs are extracted in decreasing magnitudes of explained variance, it is expected that the first few PCs account for the degradation reactions and that subsequent PCs describe noise or processes not related to product change. Therefore, the multivariate nature of the MASLT provides a powerful tool for diagnosing flaws during the study: the procedures related to storage and data acquisition should be carefully reviewed whenever it is determined that the first PCs do not account for time-related phenomena.

The Multivariate Accelerated Shelf-Life Test Algorithm. The terminology adopted here is to denote three-dimensional matrices with an underlined bold capital letter, two-dimensional matrices as bold capitals, one-dimensional matrices (vectors) as bold lower-case characters, and scalar variables in lower-case italics. The dimensions of matrices and vectors are represented as upper-case italic characters.

The MASLT is performed according to the following steps:

(1) collect the spectra in a $\underline{\mathbf{X}} \in \Re^{N \times K \times C}$ array, where N is the total number of spectra acquired per storage condition over time, K is the number of wavelengths per spectrum, and C denotes the number of storage conditions;

(2) unfold the $\underline{\mathbf{X}}$ array over the storage conditions domain to form the augmented $\mathbf{X} \in \Re^{CN \times K}$ matrix (Fig. 1);

(3) preprocess,[13] if needed, or select specific wavelengths of the augmented $\mathbf{X}$ matrix, to obtain $\mathbf{Xa}$;

(4) perform a PCA on the $\mathbf{Xa}$ matrix ($\mathbf{Xa} = \mathbf{TL}^T$), obtaining the scores ($\mathbf{T}$) and loadings ($\mathbf{L}$) matrices as well as the variance table for each PC. Select the first R PCs with higher variances (Fig. 2);

(5) split the $\mathbf{T} \in \Re^{CN \times R}$ matrix into C distinct $\mathbf{T}_c \in \Re^{N \times R}$ matrices;

(6) plot the scores of the first R PCs versus time and identify the A PCs that are time-related (Fig. 2). The time-related PCs are usually determined qualitatively by visually inspecting the kinetic charts; quantitative confirmation is obtained as follows:
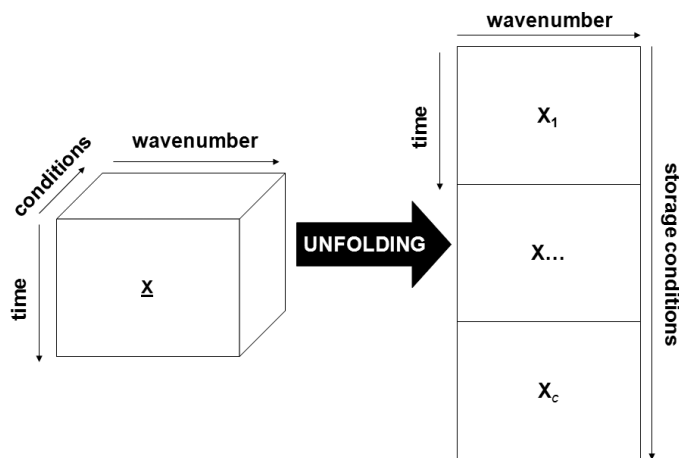
Fig. 1. Unfolding procedure of the **X** three-dimensional matrix of spectra.

Fig. 2. Pictorial representation of the MASLT.

(7) for each time-related PC, identify the reaction order and determine the multivariate kinetic parameters (k^m, E_a^m, and $\alpha_{T+\delta T,T}^m$) using the PC scores as properties in Eqs. 1 through 4 above. Plot the loadings for each time-related PC as well, and try to relate the spectral behavior to physical and/or chemical changes in the product.

Once the spectrum of an unacceptable sample is available, use the loadings to simultaneously calculate the cut-off criteria for the A time-related PCs as follows:

(8) concatenate the spectrum of the unacceptable sample into the $\mathbf{x}^T \in \Re^{1 \times K}$ vector;
(9) preprocess $\mathbf{x}^T$ using the parameters obtained in step 3 to obtain $\mathbf{xa}^T$;
(10) use the loadings matrix to calculate the cut-off criteria, i.e., the maximum acceptable scores for each time-related PC:

$$\mathbf{t}_{crit}^T = \mathbf{xa}^T \mathbf{L} \qquad (5)$$

where $\mathbf{t}_{crit}^T$ is the vector of critical scores, $\mathbf{xa}^T$ is a row vector, and $\mathbf{L}$ is the $K \times A$ loadings matrix obtained in step 4.

(11) finally, calculate the actual shelf-life of the product by projecting the cut-off score over the market condition by using the appropriate acceleration factor.

EXPERIMENTAL

One hundred flasks of body lotion were taken from the production line and split for incubation into ovens at 8, 25, 35, and 45 °C. A new sample was taken at each evaluation in order to avoid variations due to temperature fluctuations and excessive exposure to air and light. NIR spectra and sensorial assessments were performed at the initial time ($t = 0$) and weekly up to 70 days.

Reference Analyses. Sensory evaluations were performed by a 10-person trained panel.[14,15] The sensory attributes related to product degradation were fragrance character, fragrance intensity, color, viscosity (tactile), and emulsion stability.

Fragrance character is related to the hedonics of the fragrance, i.e., its characteristic scent (musky, citric, fruity, etc). Changes in character indicate that the fragrance components degraded or that an unbalanced volatilization
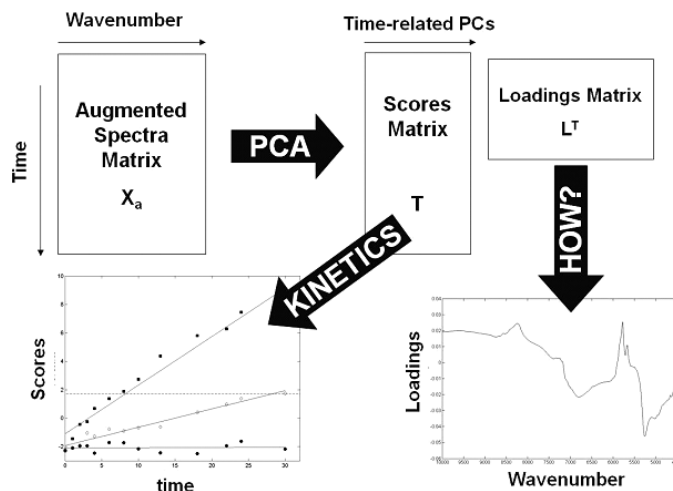
occurred. Fragrance intensity is related to the amount of fragrance released by the product. As the product degrades, fragrance is lost and its perceived intensity is reduced. Tactile viscosity is related to the amount and size of the oil droplets in the emulsion and is a key driver for consumer acceptance. Emulsion stability is related to the visual separation of phases.

Each assessor received one sample for scoring all the attributes at each assessment time and, thus, each score represents an average with nine degrees of freedom. The samples stored at 8 °C were taken as reference—for long lasting products, degradation reactions virtually stop at low temperatures—and the assessors were asked to evaluate whether the products stored at the other conditions were different from the reference according to the following scale:

0 = no difference
1 = slight difference
2 = just noticeably different
3 = different
4 = quite different

Any sample receiving an average score of 3 was considered unacceptable and taken as the cut-off for shelf-life determination. This approach relies on the fact that samples stored under harsher conditions are representative of the degradation phenomena occurring in those stored under milder conditions; the degradation just occurs at higher rates.

Moisture analyses were performed for spot checking using a Metrohm 787 KF Titrino (Metrohm, Herisau, Switzerland). Particle size determination was performed using an Olympus BX50 (Olympus Americas Inc., Center Valley, PA) microscope in conjunction with the Image Pro v4.0 (Image Cybernetics, Bethesda, MD) image analysis software.

Spectra Acquisition. Near-infrared spectra were acquired using a Büchi NIRFlex N-500 FT-NIR spectrophotometer (Büchi Labortechnik AG, Flawil, Switzerland) in the 4000 to 10 000 cm^{-1} spectral range (resolution 8 cm^{-1}; wavelength precision: 0.2 cm^{-1}; signal-to-noise ratio: 10 000:1; number of scans: 32; detector: InGaAs), equipped with a NIRFlex Solids Module and using Schott Petri dishes (ref 23 755 48 05). For avoiding spectral drift due to instrumental deviations, both the optics and the electronics signals were standardized prior to
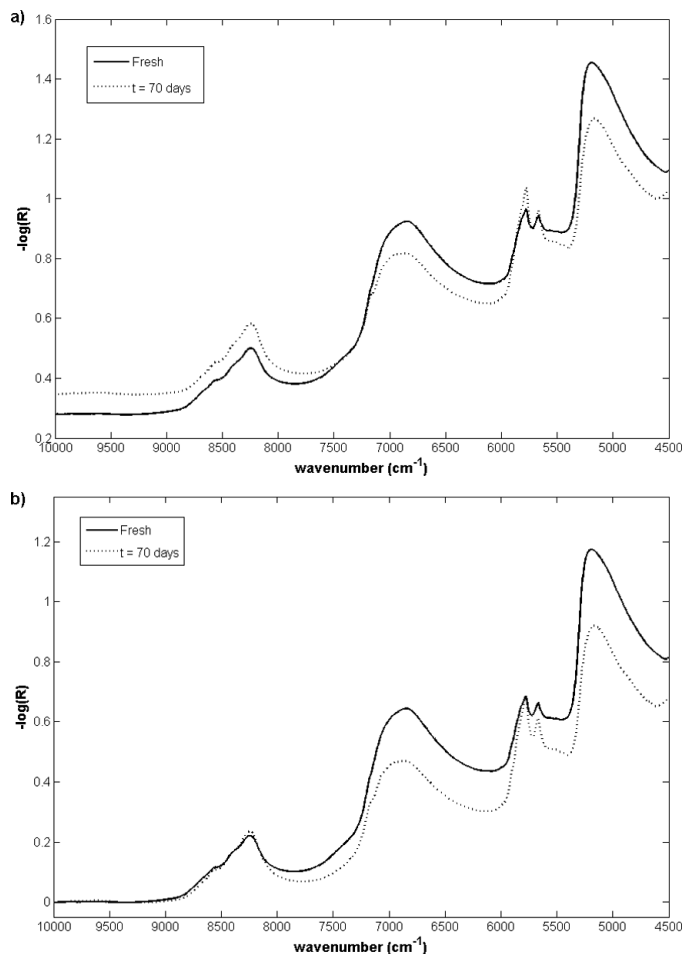
FIG. 3. Spectra of body lotion products stored for different times and at distinct conditions. (**a**) No baseline correction applied; (**b**) baseline offset removed for clarity.

performing the readings using procedures and references provided by the instrument manufacturer.

Despite the common practice of average-centering the spectra acquired by diffuse reflection prior to PCA, no spectra pre-processing was applied in this data set because it was observed that the baseline effects were related to product degradation, as will be discussed in the next section. However, the region between 4000 and 4500 cm^{-1} was excluded due to the presence of noise. Therefore, in this study $N = 11$, $K = 1376$, and $C = 4$.

Data Analysis. All the calculations were performed as described above in Matlab 7.0 R14 (Mathworks, Natick, MA) using routines developed by the authors.

RESULTS AND DISCUSSION

Figure 3 compares the spectrum of a fresh sample with that of a product stored for 70 days at 45 °C. As this temperature constitutes the most accelerated storage condition, the spectrum of the sample stored at this condition suitably represents the behavior of a product stored for long periods of time at room temperature. It can be noticed that the spectrum of the sample stored for 70 days has changed significantly in comparison to that of the fresh product. The vibration bands around 5000 and 7000 cm^{-1}, typical of water, have decreased considerably,
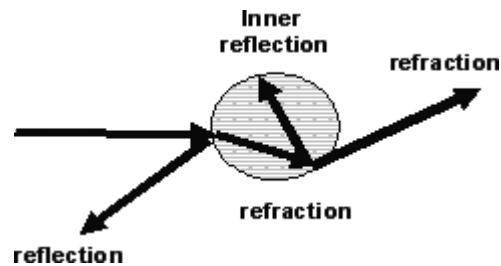

FIG. 4. Typical optical phenomena occurring at the interface of oil-in-water emulsions.

whereas the opposite effect was observed for the peak at 5600 cm^{-1}, typical of C–C bonds.[16] However, these differences in intensity cannot be explained by water loss since it was determined that the difference in moisture between these samples was smaller than 0.5%.

It can also be noticed that the baselines for the two spectra reversed positions at around 7250 cm^{-1} due to a combination of offset and differences in bias, common features of NIR spectra acquired by diffuse reflection.[16,17] In emulsions such as body lotions, the pattern of light scattering within the sample is governed by the amount, size, and shape of the droplets and by the difference between the refractive indices of the continuous and discontinuous phases: when the infrared radiation reaches the surface of an oil droplet two optical processes can occur: the light might reflect back to the continuous phase or refract into the organic phase. The same process can occur with the refracted light in the organic phase as well: once it reaches the inner surface of the droplet, the light can reflect back into the organic phase or refract to the continuous, aqueous phase (Fig. 4).[18] The net effect of these phenomena is that the optical path of the light reaching the detector can be considered the summation of optical paths in the aqueous and organic phases.

The biphasic systems of emulsions are thermodynamically unstable, being subjected to a process known as coalescence,[19] by which the oil droplets tend to collide and grow as a function of time. Moreover, the coalescence causes a significant reduction in the number of oil droplets. Indeed, it was determined that the average droplet size of the emulsion changed from 0.4 μm in a fresh sample to 5 μm in the aged sample at 45 °C. It can therefore be concluded that the baseline features observed in Fig. 3 were due to the reduction of light scattering in the emulsion. The spectral features were due to the reduction in optical path length in the aqueous phase, which was correlated with a larger optical path length in the organic phase. Both NIR features were strongly correlated with a dominant product degradation process.

Because the behavior of the baseline brought relevant information with regards to product degradation that is strictly linked to emulsion stability, no baseline correction was applied to this data set for performing the MASLT calculations.

The u-PCA yielded two time-related PCs that accounted, respectively, for 98% and 1% of the variance in the dataset. The loadings plots for these PCs are shown in Fig. 5. It can be noticed that PC1 was strongly influenced by the average spectrum, mostly capturing baseline features (which explains its ability to capture most of the variance in the dataset). PC2 captured spectral changes related to the organic phase, which can be explained by the increase in optical path length of this phase over time.
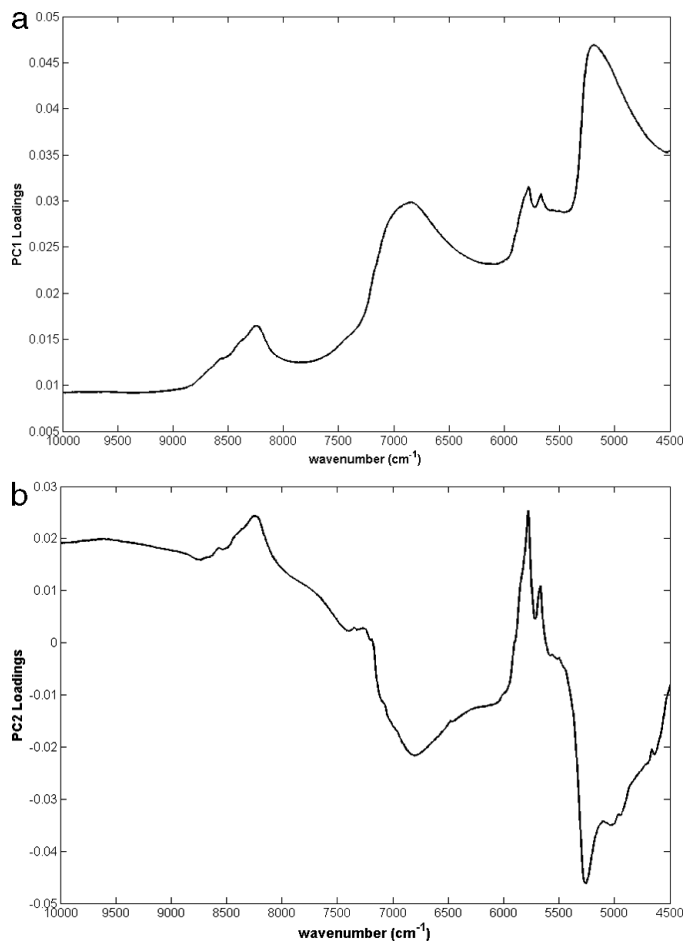
FIG. 5. Loadings plots for PC1 and PC2.

FIG. 6. Kinetic charts of the scores of samples stored at (●) 8, (◇) 25, (□) 35, and (∗) 45 °C. The dashed lines represent the cut-off criteria for each PC and the solid line highlights the differences in kinetics followed by the scores of each PC at 45 °C.

Care should be taken when performing preprocessing on NIR spectra for shelf-life studies because baseline features might bring relevant information on product stability and further contribute to the interpretation of degradation mechanisms: as has been herein demonstrated, the baseline offset and bias, related to droplet size and number, were significantly related to emulsion stability.

Figure 6 shows the kinetic charts of the scores of both time-related PCs. Notice that, for both PCs, the samples stored at 8 °C and 25 °C did not present major differences in the degradation profiles during the accelerated study because body lotions are indeed long-lasting consumer goods. Only minor variations were observed in the scores of products stored at 8 °C over time, which corroborates the assumption commonly raised in performing sensory analysis, that the degradation reactions were virtually stopped at this condition.

Because harsher storage conditions represent samples stored for longer periods at market condition, the samples stored at 45 °C were used for determining the scores' kinetics order. It was determined that the PC1 scores followed pseudo-first-order kinetics while PC2 scores followed pseudo-zero-order kinetics. The multivariate rate constants (k^m), as well as the multivariate acceleration factors ($\alpha_{T,25}^m$) and activation energies (E_a^m), are shown in Table II. Notice that despite presenting degradation reactions of different kinetic orders, the acceleration factors and the activation energies for both PCs were quite similar. Since baseline and the spectral changes over time were a function of
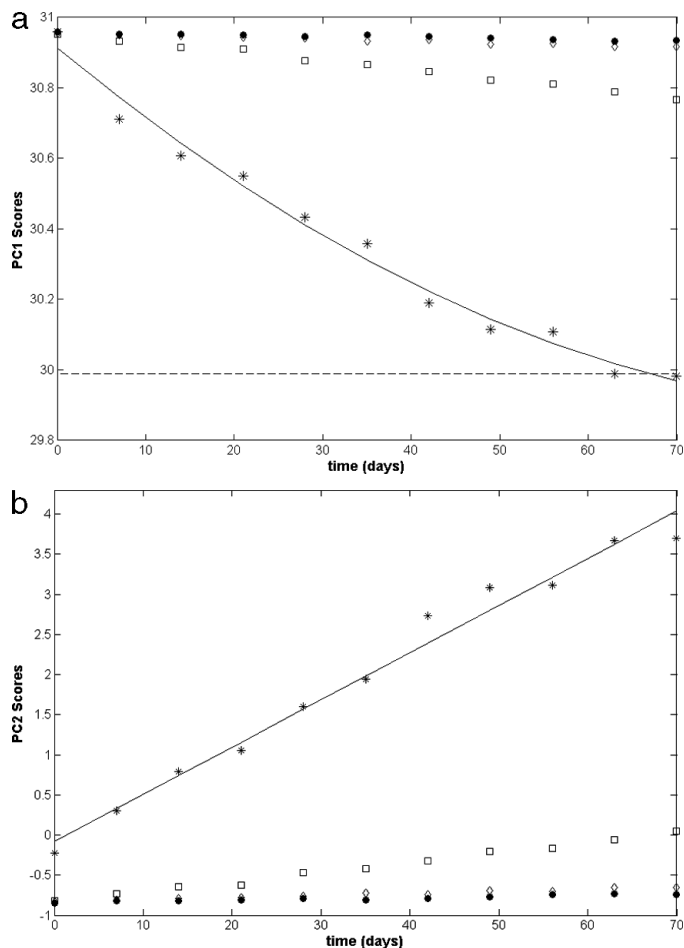
the same degradation process, the observed correlation between the kinetic parameters of both PCs was expected.

Table III shows the sensory evaluation for the quality parameters of the body lotion for products stored at 45 °C; samples stored at other temperatures did not present any

TABLE II. Multivariate shelf-life figures for PC1 and PC2.[a]

Storage conditions (°C)	Rate constants k^m (day^{-1})	Acceleration factors ($\alpha_{T,25}^m$)	Activation energy E_a^m (kJ·mol^{-1})
PC1			
8	$1.1 \times 10^{-5} \pm 1 \times 10^{-5}$	...	
25	$1.8 \times 10^{-5} \pm 1 \times 10^{-6}$	...	
35	$8.5 \times 10^{-5} \pm 2 \times 10^{-6}$	4.5	73 ± 8
45	$4.2 \times 10^{-4} \pm 2 \times 10^{-5}$	25	
PC2			
8	$1.6 \times 10^{-3} \pm 2 \times 10^{-3}$	...	
25	$2.7 \times 10^{-3} \pm 2 \times 10^{-4}$	...	
35	$1.2 \times 10^{-2} \pm 3 \times 10^{-4}$	4.4	70 ± 9
45	$5.8 \times 10^{-2} \pm 3 \times 10^{-3}$	22	

[a] Since rate constants and activation energies were calculated through linear regressions, their values are expressed as coefficient ± standard error of coefficient.

TABLE III. Sensory evaluations for samples stored at 45 °C.

Time (days)	Scores (average)				
	Fragrance character	Fragrance intensity	Color	Viscosity (tactile)	Emulsion stability (visual)
7	0.6	0.2	0.0	0.1	0.1
14	0.5	0.2	0.2	1.1	0.1
21	0.8	1.2	0.5	1.3	0.1
28	0.8	1.3	1.1	1.5	0.3
35	0.9	1.4	1.2	1.7	0.2
42	1.1	2.0	0.9	1.7	0.3
49	1.1	2.2	1.2	1.9	0.6
56	1.3	2.8	1.5	2.2	0.8
63	1.5	3.0	1.3	2.1	1.1
70	1.8	3.3	2.1	2.3	1.0

significant sensorial variation during the whole accelerated shelf-life study. The sample stored for 63 days received an average score of three for fragrance intensity and, since this is a key attribute of consumer acceptance, the spectrum of this sample was taken as the cut-off limit (dashed line in Fig. 6) for determining the shelf-life of the product.

It was a coincidence that the sample stored for 63 days received an average score exactly equal to 3. It is indeed usual, in practical shelf-life studies, for samples stored for a given period to be scored higher than the cut-off criterion in a specific quality parameter. In such cases, the equivalent spectra should be calculated by interpolation and Eq. 5 should be used for determining the cut-off score value for each time-related PC. Nevertheless, since shelf-life studies of consumer goods are usually not extremely precise, and because the sensory evaluation is usually of low resolution, there is no need to apply sophisticated regression techniques on the scores. Usually one might rely on linear or polynomial interpolation techniques, but splines can also be applied depending on the specific dataset and on the objectives of the study.

The findings presented herein demonstrate that NIR spectroscopy was indeed effective in detecting emulsion stability changes over time and that these changes were related to fragrance perception, noticeably fragrance intensity. Fragrances possess components that might stabilize emulsions.[20] However, as soon as the oil droplet size and the liquid–liquid crystal phases of the emulsion change, the olfactory profile of the product might change accordingly, depending on the compositions of the fragrance and on the emulsion system.[21] In the present study, no change in the partition coefficient of the fragrance compounds occurred since no change in fragrance character was observed by the sensory panel; changes in the partition coefficients would lead to the unbalanced release of different components, leading to the perception that the fragrance hedonics had changed. The detected change in fragrance intensity is probably due to a decrease in the barrier properties of the oil-in-water emulsion as the oil droplets became larger and lower in number. Further, the higher the storage temperature (which decreased the aqueous phase viscosity and increased fragrance volatilization), the larger the fragrance loss over time.

Once the kinetic parameters and the cut-off criteria were known, the shelf-life of the body lotion stored at the market temperature (25 °C) was finally calculated by projecting the cut-off time of the sample stored at 45 °C (63 days) over the scores of PC2, using the most conservative acceleration factor

$(\alpha_{45,25} = 22)$:

$$\text{shelf-life}_{25} = \alpha_{45,25} \times \text{time}_{\text{crit},45} = 22 \times 63$$
$$\cong 1380 \pm 120 \, \text{days}$$

which corresponds to 3 years and 9 months $\pm$ 4 months. If the scores of PC1 were used instead, a slightly longer shelf-life would be determined: 4 years and 3 months $\pm$ 4 months.

The shelf-lives of similar body lotion products, determined via the conventional sensory and physical chemical measurements, are 3 years. The result obtained by using NIR spectroscopy can thus be considered suitable since it is common practice in industry to establish more conservative estimates of shelf-lives for consumer goods. No shelf-life study is either absolutely representative or precise; for instance, sources of variations such as transportation and temperature oscillations are usually not included in the shelf-life tests.

CONCLUSION

The procedure presented herein constitutes a novel approach for determining the shelf-life of products using NIR spectroscopy and chemometrics. It opens the opportunity for studying possible applications not only for the cosmetics industry but for pharmaceutics, foods, agriculture, petrol, fuel, and plastics industries, as well as any other transformation activity that needs to perform shelf-life studies prior to releasing innovative products to the market.

The specific application disclosed in this work has successfully demonstrated how NIR spectroscopy can be applied for determining the shelf-life of products since it led to the same conclusions as those obtained by the conventional time- and resource-consuming techniques. This study also constitutes an example of how knowledge from diverse fields such as analytical chemistry, spectroscopy, physical chemistry, and sensory analysis can be used for delivering significant benefits to the industry. In this example, the NIR spectroscopy provided meaningful quantitative information for performing kinetic calculations and mechanistic interpretations, the sensory analysis supplied a cut-off criterion that was representative of consumer perception, and chemometrics, as proposed by the MASLT algorithm, provided the mathematical basis for merging the information together.

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