

Assessment of the prediction efficiency of three simulation software concerning the conformity of compostable shoppers from a packaging industry before TÜV verification

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INTRODUCTION

In order to go towards more eco-friendly life conditions, in Italy since 2006, plastic-based shoppers, have been progressively replaced by the compostable ones. Nowadays plastic-based shoppers are considered illegal and only compostable ones are accepted. They are produced by several packaging industries widespread throughout Italy including Mecplast that was involved in this study. Compostable shoppers must meet specific requirements, such as minimum renewable raw material content of at least 40% (fruits and vegetables bags), a thickness of 15-30 my depending on the cocktail ingredients involved in the production and suitability for food use.¹ These specifics are verified to grant to the producers a conformity certification, currently issued by TÜV ITALIA (ex Vincotte). Once the certification "OK compost" has been granted, certified industries products must undergo regular verification of chemical composition by means of Fourier Transform Infrared (FTIR) spectroscopy.

Analytical techniques and data processing methods

FTIR spectroscopy is extensively applied for routinely analysis in several industrial sectors including packaging, because it doesn't require sample preparation or use of chemicals or consumables, it is non-destructive, operator friendly, fast, reliable, precise and low cost. Spectral data of a set of samples are arranged in very large matrices. To get reliable information from spectral data matrices the so called Principal Component Analysis (PCA) is usually adopted. PCA is a chemometric tool, able to elaborate a orthogonal conversion of a great number of possibly correlated variables, into a set of values of few linearly uncorrelated variables (Principal Components) endowed with the maximum of predictive information. To work up PCA, many statistic simulation software, such as Analytics, R, MatLab, JMP etc. are commercially available.

THIS WORK

In this study, due to their simulative power, even if not among the CAE software, JMP, MatLab and R have been put under investigation, to assess their efficiency in working up PCAs on FTIR spectral data matrices of different complexity and size and in providing useful predictive information. A set of samples of shoppers for food packaging have been used for developing this project. On the request of Mecplast, a food packaging industry located in Savona, Liguria (Italy), the desired information concerned the prediction of the possible conformity of a new production of compostable shoppers before TÜV verification.

Collaboration and "exchange of pleasures" with Mecplast

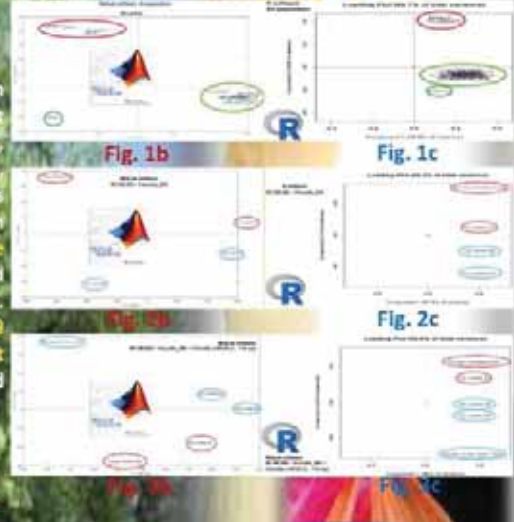
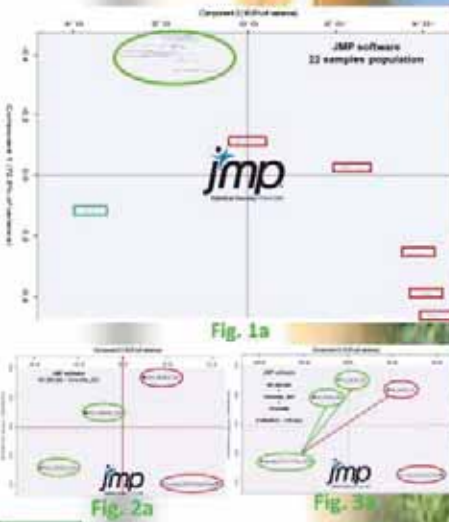
Thanks to the providential, born by chance, collaboration with Mecplast, unknown samples on which acquiring FTIR spectra, to include into FTIR data matrices obtained from a population of reference samples were available. Therefore the matrices on which to perform PCAs by selected software, were built up as follows.

MATERIAL & METHODS

A set samples of 15 films, was created by collecting shoppers with TÜV certification from different markets in Genoa, Italy. In this set were furtherly included: a certificated film produced by Mecplast, in 2017 (namely Vincotte_303), a completely not biodegradable, irregular PET-based film (namely PE_shopper), STARCH, as reference for a totally compostable natural material and a film with PLA>40% and thickness <15 my (namely Vincotte_400<15my), representing an ideal compostable film as standard reference. The total Reference population resulted of 19 samples. FTIR spectra were acquired in triplicate on all the population of 19 samples and on the three new samples provided by Mecplast (namely M1, M2, M3), unknown to us for composition and thickness. PCAs should have provided the information.

Data matrices built up for PCAs

Two small matrices, one collecting FTIR data of four samples, i.e. M1, M2, M3 and Vincotte_303, in the other, the FTIR data of five samples, i.e. M1, M2, M3, Vincotte_303 and Vincotte_400<15my plus a large matrix collecting FTIR data of all the 22 samples, were built up and JMP, MatLab and R were used to work out PCAs on them.



Conformity Prediction

RESULTS & DISCUSSION

Chemical Composition of M samples

As confirmation of the assumption in the left green box, from their position in PCA (PC1, Fig. 3a, 3b, 3c), M2 and M3 resulted of equivalent composition and similar to the sample Vincotte_400<15my, while M1 resulted different from M2 and M3 and more similar to Vincotte_303. As already noticed, all PCAs worked up by JMP provided this prediction, thanks to the remarkable samples separation achieved in every case. Differently, PCAs elaborated by R and MatLab on the large data matrix of 22 samples is not useful to get this information, due to the very poor samples separation provided in this case (Fig. 1a and 2a). Only in the PCAs worked out from the smaller data matrices (Fig. 2b, 2c, 3b, 3c), this prediction is readable (PC1, Fig. 2b, 2c, 3b, 3c). Finally, MatLab was slightly more performant than R elaborating PCAs that, even if not informative, show a bit of samples separation also in Fig. 1a.

Thickness of M samples

As confirmation of the assumption in the left green box, from their position in PCA (PC2, Fig. 3a, 3b, 3c), M3 resulted different from it for thickness. M3 locations, always more closer than M2 and M1 to the Vincotte(PLA>40%;<15my), predict a thickness of about 15 my for M3 and different values (Mecplast made known 30my) for M2 and M1. As in the previous cases, JMP resulted the most performant software in processing FTIR data for PCAs, and in providing this prediction in all PCAs containing the reference sample (Fig. 1a and 3a). Concerning MatLab and R, only in the PCAs worked out on the small data matrix from 5 samples, prediction about samples thickness, is readable.

As observable by their position both on PC1 and on PC2 (Fig. 1a, 1b) and on PC2 (Fig. 2a), all the new films from Mecplast resulted to make part of the population of compostable films taken as references. As Figures show, in PCA worked up by JMP and MatLab, this prediction is readable on two Principal Components (PC1 and 2), while in PCA only in one (PC2). R worked up PC1, with less separation of the samples than JMP and MatLab, no separation is appreciable in PC1 and therefore no prediction can be extracted (Fig. 1a). JMP performed the best PCA for separation of the samples. Good separation is evident also within a cluster, thus providing more predictive information. In this regard, M2 and M3 inhabit the same position in PC1, that could mean same composition, but different in PC2, that could mean different thickness. Confirmation of these assumptions has been obtained observing others PCAs (Fig. 2a, 3a). The TÜV OK compost sample appears rather far from the compostable population!!!! It makes think...

CONCLUSIONS & ENVIRONMENTAL CONCERNS

In order to prove before official verification by TÜV eligibility for certification of new compostable shopper of Mecplast productions were achieved by PCA-assisted FTIR analysis in fast and low cost way. JMP, MatLab and R simulation software were selected to work out PCAs on FTIR data matrices. JMP resulted the most efficient in developing PCAs with a remarkable samples separation also within the clusters allowing to achieve the maximum of information on all the data under study. R was the most performant. R and MatLab proved to be able to elaborate informative PACs when applied on small matrices, but failed when applied on the large data matrix from all samples. With great disappointment, from the PCAs elaborated, has been highlighted that only in the restrict zone of Genoa investigated, up to 4 samples on a population of 20 (20%) despite market with TÜV certification as compostable shoppers, resulted to be out of the compostable population according to the requisites established by current law and required instead similar and higher prediction to the non-degradable, frequent plastic-based PE SHOPPER. This fact should represents a concern and an outstanding problem that needs to be solved.



[1] Law of 3 August 2017, n. 123, in association to the UNI EN 13432 standard and to the UNI CEN/TS standard. [2] Principal Components Analysis, P. Wallisch, in MATLAB for Neuroscientists (Second Edition), 2014.