Original Article

Evaluation of FTIR and multivariate data analysis for the control of medical devices

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Abstract

Verification of sterilization number of medical devices is one of the main objectives to control its quality and ensure the protection of patients. The objective of this study is to investigate the capability of an automatic tool based on the combination of mid-infrared spectroscopy with a mathematical and statistical algorithm to estimate the number of sterilization cycles of medical pipes. Data analysis is performed by three main methods of pattern recognition: principal component analysis (PCA), support vector learning regression (SVR), and partial least squares regression (PLSR). The result obtained shows high performance capabilities for the prediction of sterilization cycle number. These technologies could be successfully applied in hospitals to ensure the quality of medical devices.

Keywords: medical devices, sterilization, spectroscopy, data analysis

DOI: 10.47750/pnr.2022.13.S04.125

INTRODUCTION

Reusable medical devices are a potential source of nosocomial infections(Healthcare Equipment as a Source of Nosocomial Infection: A Systematic Review - Journal of Hospital Infection, n.d.). Faced with this risk, it is necessary for hospitals to control the sterilization process(Schabrun & Chipchase, 2006; Wenzel & Edmond, 2001). Sterilization is a complex, multi-step process that renders a product sterile and must maintain this state for a specified period of time. Aspiration pipes for suction systems and various drainages: Bronchial, nasopharyngeal, gastric, thoracic, and various drainages in surgery. These devices are to be changed between each patient and must be replaced by others that are disinfected and sterile, to avoid infection of patients who will reuse them afterward(ASHP Guidelines on Quality Assurance for Pharmacy-Prepared Sterile Products, n.d.). In the hospital environment, the sterilization of these materials can be done by two processes; low-temperature sterilization processes which are expensive for some, or dangerous for others use toxic sterilizing agents (ethylene oxide, formaldehyde ...), or by another steam sterilization process which is safe and widely used with a sterilization cycle whose tray is fixed at a temperature of 121°C for 20 minutes.

These aspiration pipes are generally made of silicone and tolerate sterilization temperatures, moreover, repeated sterilization damages these aspiration pipes and the disinfection step becomes difficult due to the appearance of micro cracks that will not be eliminated by this step, so the effectiveness of sterilization is not guaranteed(Janoly-Dumenil et al., 2005).

The objective of this work is to determine the number of sterilization cycles undergone by a suction tube using FT-MIR spectroscopy and multivariate statistical algorithmes, in order to predict its duration of use to avoid any risk of contamination of patient contamination.

Materials And Methods

Samples preparation

The sterilizer pipes are essentially analyzed using mid-infrared spectroscopy, each sample is analyzed according to the number or cycle of sterilization. then spectral treatments were applied to eliminate the effects of humidity and CO_2.

Multivariate data analysis

Most analytical study involve many variables. Analysts take into account multiple performance measures and associated metrics when making policy decisions. In cases of problems that involve three or more variables, the results are inherently multivariate and require the use of multivariate data analysis.

Principal component analysis(PCA)

Principal component analysis is part of the group of multidimensional descriptive methods known as factorial methods (descriptive, unsupervised)(El Orche, Mamad, et al., 2021). PCA searches for the spatial directions in which individuals are most dispersed, assuming that these directions are the most interesting. In this way, once these directions are determined, it produces n new orthogonal axes named "principal components" or "PCs" which represent the linear combinations of the initial variables. Principal component analysis is performed by applying one of the many algorithms available(Jolliffe, 2002). All of them aim to create a set of linear combinations of the original variables in such a way that the initial matrix (X) is decomposed into two new matrices, one named matrix of scores (T) and the other named matrix of loadings (P) plus residue matrix according to :

$X=T*PT+E$ (1)

Partial least square regression (PLS)

PLS regression is an analytical approach widely used in chemometrics to find a linear relationship between two matrices of variables X and response Y(El Orche, Adade, et al., 2021; El Orche et al., 2020; Elhamdaoui et al., 2020). It aims to model simultaneously the variability of the two matrices by calculating latent variables that maximize the total variability contained in the two matrices as well as their correlation. This operation often involves performing a decomposition based on the Nonlinear Iterative Partial Least Squares algorithm, of the 2 matrices X and Y with the condition that the latent variables, T, extracted from X are as correlated as possible with the latent variables, U, extracted from Y(Abdi, n.d.; Nengsih et al., 2019; Orche et al., n.d.).

Model of X: $X = T*PT +E$ (2)

Model of Y: $Y = U*CT +F$ (3)

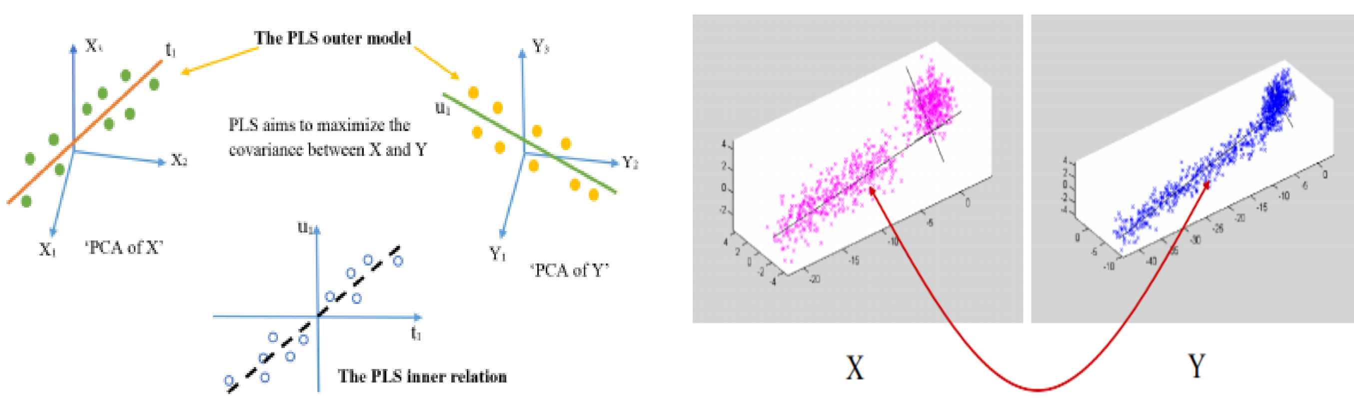

Figure 1: illustration of PLS operation which consists in maximizing the correlation between the Latent Variables t and u(El Orche et al., 2020; Madakyaru et al., 2019).

Support vector machine regression(SVMR)

SVM or Support Vector Machines is among the most common and broadly used algorithms for processing classification problems in machine learning(El Orche, Mamad, et al., 2021). However, the use of SVMs in regression has not been well documented. However, this algorithm recognizes the presence of non-linearity in the data and produces an effective prediction model. Support vector machines are a supervised learning model with related learning algorithms that analyze the data needed for classification and regression assays. In support vector regression, the straight line involved to adjust data is called a hyperplane. Support vector regression is a supervised learning algorithm which is applied to predict discrete parameters. Support vector regression follows the same principle as SVMs. The fundamental concept of SVR is to determine the most suitable line. In the SVR, the best suitable line is the hyperplane that contains the maximum number of points(Johnson et al., 2022).

Results And Discussion

Figure 1 shows FT-MIR spectra of pipe samples. Two main absorbance at 785, 1005cm-1 respectively associated with a ring C-H out of plane banding and vibration of aromatic ring. Tree other weak bands were observed at 1259 cm-1 ,1466 cm-1 and 1592cm-1 , caused respectively by C-N amide III band, stretching –C-O and C=N stretching(Mecozzi & Sturchio, 2017).

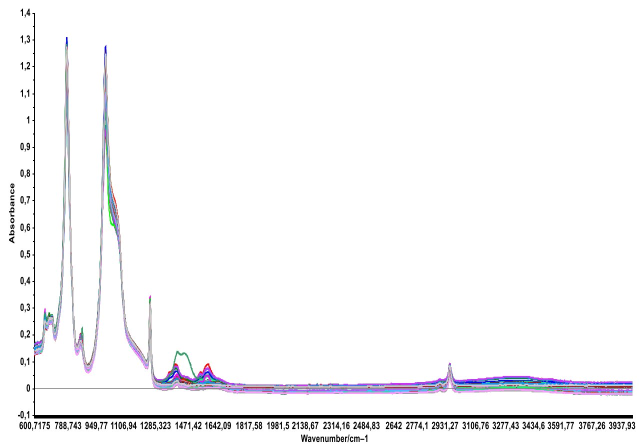

Figure 2: FT-MIR spectra of pipes samples.

Principal Component Analysis

PCA was applied to the spectral data in order to have an idea about the structure of the data and identify outliers. PCA results show that the first two components account for 86% of the total variability of the data. According to the score plot, we can distinguish that there are three classes, suggesting that the samples belonging to both groups have common FTIR properties.

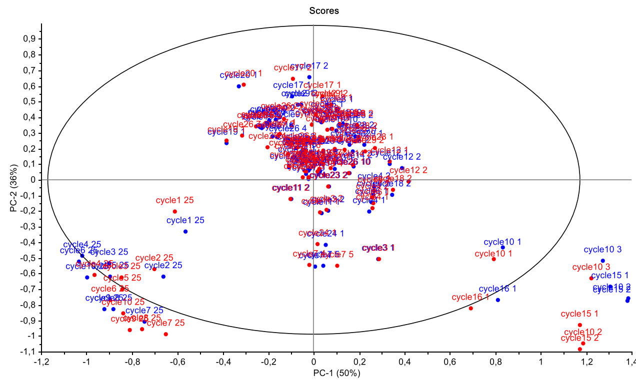

Figure 3: PCA score plot of the two first principal component.

Partial Least Square Regression

In order to predict the number of pipe sterilization cycles in the range 2-26, a partial least squares regression model and a machine support regression model were constructed using the FTIR spectra of all samples.

For PLS regression The determination of the optimal number of latent variables required to predict the number of sterilization cycles was performed based on the cross-validation root mean square error and R-square values calculated according to the "Leave One Out" cross-validation procedure(Abdi, n.d.; Westerhuis et al., 2008). For this study, 14 Latent Variables have been selected, which resulted in an RMSEP value of 3.89.

In fact, a correlation coefficient R-square of 0.92 obtained using PLS regression which demonstrates good linearity of the model and a satisfactory relationship between actual and predicted number of sterilization cycles of pipes.

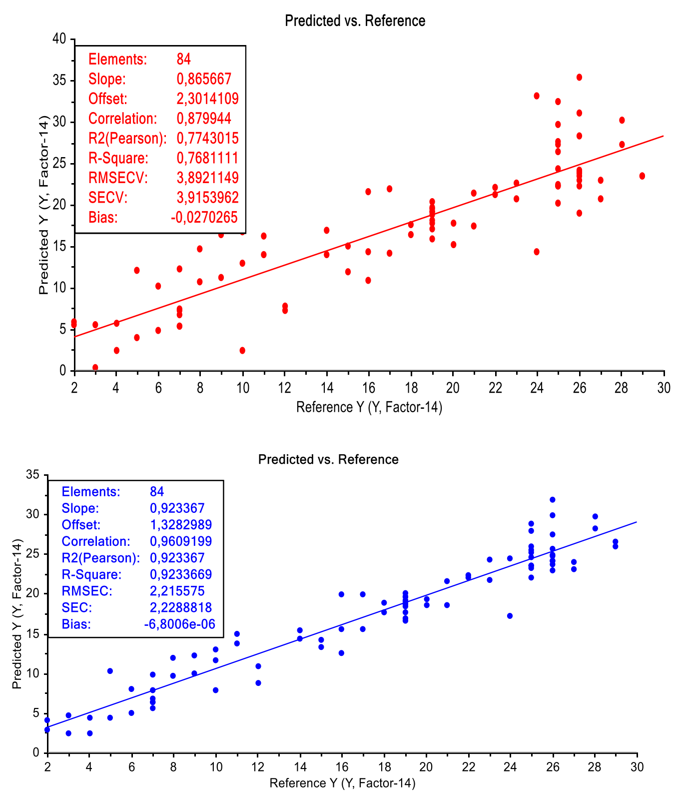

Figure 4: Graph of predicted value versus real sterilization number using PLS regression (Blue: calibration and red: Cross-validation)

Support Vector Machine Regression

The main goal of the SVR model is to perform linear regression by plotting spectral data in high-dimensional space and building a linear decision function in large dimensional space.

The use of the SVR shows an acceptable capacity for the determination of the number of sterilization cycles. These capacities are shown by the high value of R-square 0.79 and the low value of RMSEC 5.09. The examination of this model by the cross-validation shows an R-square value of 0.59 and an RMSECV of 6.07. These values are considered very low compared with those found by the PLS regression.

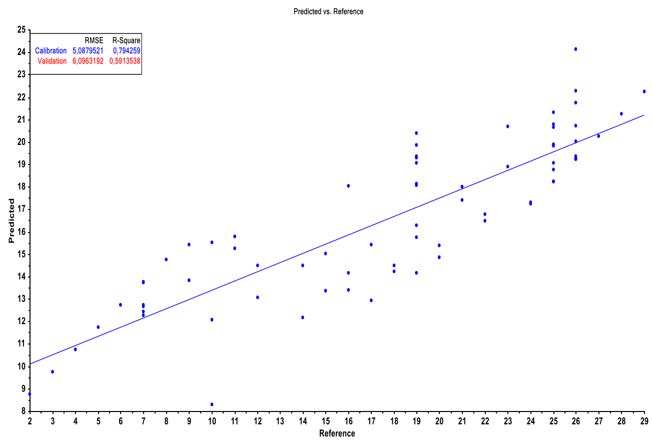

Figure 5: Graph of predicted value versus real sterilization number using SVM regression.

Conclusion

This study presents a statistical approach based on the exploitation of FT-MIR spectral data by chemometric algorithms in order to control the number of sterilizations of tubing used in medical treatment and operation.

The use of PLS and SVM regression shows an acceptable capability for the prediction of sterilization numbers.

The results show that the proposed protocols are effective for monitoring the sterilization of pipes within the hospital. In future work, the proposed approach will be extended to take into account the chemical nature of the pipes and also by the application of mathematical treatment to eliminate undesired signals in order to improve the quality of prediction of the constructed models.

Acknowledgement

Thank you editors, brothers and friends to assist this publishing.

Conflicts Of Interest

There is no conflict of interes

Authorship Contribution Statement

Mustapha Bouatia: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Data curation, Writing – original draft, Writing – review & editing. Aimen El Orche: Investigation, Formal analysis, Data curation, Writing – review & editing. Amine Cheikh: Conceptualization, Methodology, Writing – review & editing, Supervision, Funding acquisition. Hafid Mefetah : Supervision, Funding acquisition Khalid karrouchi : Conceptualization, Miloud El Karbane : Conceptualization .

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