# Chemical imaging and quantification of RDX/PETN mixtures by PLS applied on terahertz time-domain spectroscopy

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***Abstract*—Chemometric analysis was applied on terahertz absorbance 3D images, in transmission. The goal is to automatically discriminate some explosives on images and quantify mixtures of RDX/PETN in the frequency range of 0.2 – 3 THz. Partial Least Square (PLS) was applied on THz absorbance multispectral images to quantify individual product inside pure samples and mixtures at each pixel on the image. Then the best score obtained is used to display the samples' images and provide the optimal frequencies combination for recognition purpose.**

## I. INTRODUCTION

Terahertz spectral-imaging is an imaging technique that utilizes the wave in the terahertz region of the electromagnetic spectrum (3-0.03 mm; 0.1-10 THz) [1]. It was investigated in different fields such as biology, pharmaceutical, security fields, etc., and allows getting physical and chemical information about the inspected samples by getting the dielectric response over several decades of frequencies.

On the other hand, chemometrics technics showed powerful capability in data analysis for discrimination, identification or quantitation. As well as in terahertz science, chemometrics was successfully applied on spectroscopy [2] and on imaging [3] for various purposes.

Partial least square (PLS) is one of the chemometrics multivariate analyses used to get chemical information on multispectral data and to predict the amount of products in samples. Different studies demonstrated the good ability of PLS applied on THz spectra for quantification of different chemical substances [4].

In the context of transportation security and in the aim of not only identify some explosives but also to predict their exact amount in the terahertz domain, we applied PLS algorithm on multispectral terahertz images. This study was made in order to quantify two explosives cyclotrimethylenetrinitramine (RDX) and pentaerythritoltetranitrate (PETN) in pure state and in mixtures on each pixel of THz multispectral images.

## II. RESULTS

Three different pellets of 400 mg total weight and 13 mm diameter were imaged for this study. The first and second pellets contain 80 mg RDX and PETN respectively. The third pellet contains 40 mg RDX and 40 mg PETN. Also, 36 pellets of pure RDX, pure PETN or mixtures, with different amounts ranging from 2 mg to 100 mg. For all the pellets, polyethylene (PE) was used as a binder. Terahertz measurements were obtained from time domain spectral imager, TPS spectra 3000 from Teraview, working in transmission mode. The selected frequency band is 0.2-3 THz. Then, a Fast Fourier Transform leads to extract the absorbance spectra using PE measurements as reference. The resulted image has a size of 39*13 $mm^2$ which correspond to a 66*22 pixels. The 3D matrix of data was transformed in a 2D matrix PxF, where P corresponds to 1452 pixels in the image and F corresponds to 486 frequencies. It should be mentioned that each F vector corresponds to an entire image. Then, a PLS model was build where 622 absorbance spectra of the 36 pellets was used to calibrate the model, and the 2D matrix, unknown for the model, was used in order to predict the amount of RDX and PETN on each pixel of the 1452 on the entire image. The results show good ability of the model in prediction, with a RMSE lower than 4 mg for the entire 400 mg pellet. We will also present our model, the results in term of scores, loadings, root mean square error (RMSE) and the spatial repartition of predicted values on the image.

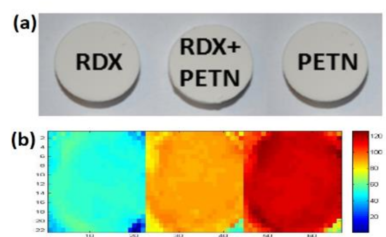


**Fig 1:** (a) Photo of three different pellets of 400 mg total weight constituted respectively of 80 mg RDX, 40 mg RDX/40 mg PETN and 80 mg PETN, (b) image of the predicted pixels: blue, orange and red correspond to 80 mg RDX, 40 mg RDX/40 mg PETN and 80 mg PETN respectively with an RMSE less then 4mg.

## III. SUMMARY

In this study we showed the ability of PLS analysis applied on THz multispectral absorbance images, in quantification of RDX and PETN explosives inside mixtures, not only from one THz spectrum measurement, but on an entire multispectral image. So with this procedure, we can detect, quantify and display explosives hidden inside pellets.

## REFERENCES

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