

Electronic tongue sensing of explosives and its mixtures

Xavier Cetó, Andreu González-Calabuig, **Manel del Valle**

Biosensors Group, Department of Chemistry, Universitat Autònoma de Barcelona, Spain

manel.delvalle@uab.cat

With the surge of international terrorism and the increased use of explosives in terrorist attacks, law enforcement agencies throughout the world are faced with the problem of detecting hidden bombs in luggage, mail, vehicles, and aircraft, as well as on suspects.

Nowadays, this has become a major analytical problem, which requires highly sensitive, specific, fast and reliable field-deployable detection strategies [1]. On that account, electrochemical sensing represents a promising solution for on-site explosive detection given the inherent redox activity of commercial explosives, which makes them ideal candidates for voltammetric monitoring.

Nevertheless, despite the initial attempts made to voltammetrically detect the aforementioned compounds employing different types of electrodes and techniques [2], even achieving its detection at very low concentration levels, further work is still required to accomplish the correct identification and quantification of explosives and its mixtures.

A chief challenge encountered within these analysis is the discrimination between individual compounds present, given that the voltammetric signals produced by these electrochemical methods correspond to a global overlapped, multiple peak voltammogram; i.e. there is a lack of specificity or identification of differentiated peaks for each of the compounds (Figure 1). Thus, in order to determine more accurately which type of explosive combination is used, providing the ability to discern between different explosive compounds in a mixture is necessary, especially for security issues.

In this sense, the combination of electrochemical methods with chemometric tools such as Principal Component Analysis (PCA) or Artificial Neural Networks (ANNs) can help to overcome this limitation [3], by identifying and processing the electrochemical fingerprint shown by the explosive mixture. Hence, arising as a powerful alternative to classical methods for the identification of explosive compounds [4, 5].

The followed approach, known as Electronic Tongue (ET) [6], consists in the coupling of an array of sensors with marked mix-response towards the desired species, plus a chemometric processing tool able to interpret and extract meaningful data from the complex readings, relating them with their analytical meaning. For its implementation, first it is needed an appropriate sensor array with some cross-sensitivity between them, which allows the simultaneous determination of a large number of species, while the chemometric treatment of the data allows the resolution of the interferences, drifts or non-linearity obtained with the sensors [7]. Moreover, the data processing stage may offset any matrix or interference effect from the sample itself. Thus, with this methodology, it is possible to achieve a parallel determination of a large number of different species, while any interference effect is solved using these advanced chemometric tools.

Preliminary attempts to distinguish common explosive compounds such as TNT, RDX or PETN using a single bare screen-printed carbon electrode (SPCE) were performed; while in a second attempt, a miniaturized array of graphite, gold and platinum sensors was used, which allowed also the detection of peroxide-based explosive compounds such as TATP. The method proposed herein couples field-deployable

electrochemical measurements with multivariate calibration models obtained by ANNs, with the aim to examine the potential of a voltammetric device for the detection of explosive compounds and mixtures using either qualitative discrimination (Figure 2) or quantitative determination (Figures 3&4).

Figures

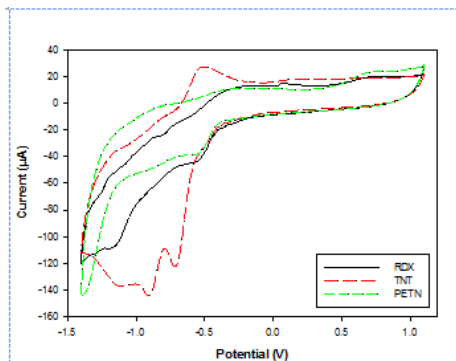


Figure 1: Example of the different voltammograms obtained with the SPCE for $50 \mu\text{g}\cdot\text{mL}^{-1}$ standard solutions of three common explosive pure compounds.

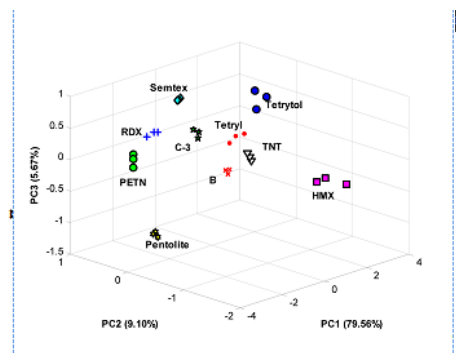


Figure 2: Score plot of the first three components obtained after PCA analysis.

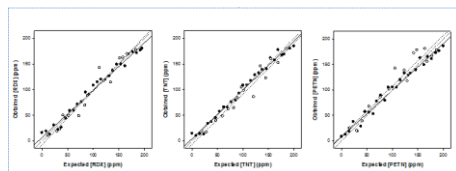


Figure 3: Modeling ability of the optimized ANN for the single SPCE sensor. Comparison of obtained vs. expected concentrations of ternary mixtures of RDX, TNT and PETN, both for the training (●, solid line) and testing subsets (○, dotted line). Dashed line corresponds to theoretical.

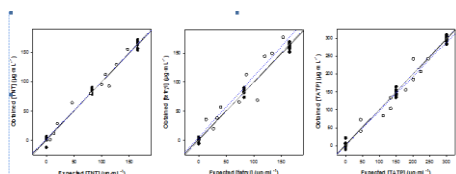


Figure 4: Modeling ability of the optimized ANN for the miniaturized sensor array. Comparison of obtained vs. expected concentrations for ternary mixtures of TNT, tetryl and TATP, both for the training (●, solid line) and testing subsets (○, dotted line). Dashed line corresponds to theoretical.

References

- [1] J. Wang, *Electroanalysis*, 4 (2007) 415
- [2] J. S. Caygill, F. Davis, and S. P. J. Higson, *Talanta*, 0 (2012) 14
- [3] Y. Ni and S. Kokot, *Analytica Chimica Acta*, 2 (2008) 130
- [4] X. Cetó, A.M. O'Mahony, J. Wang, M. del Valle, *Talanta*, 107 (2013) 270
- [5] A. González-Calabuig, X. Cetó, M. del Valle (*Talanta*, submitted)
- [6] M. del Valle, *Electroanalysis*, 14 (2010) 1539
- [7] A. Riul Jr, C. A. R. Dantas, C. M. Miyazaki, and O. N. Oliveira Jr, *Analyst*, 10 (2010) 2481