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Available Technologies

Chemometric Characterization and Classification of Unknown Vapors

SUMMARY

Presented here is a method for taking the data generated from an array of responses from a multichannel chemical sensor instrument, and determining the characteristics of a chemical in the sample without the necessity of calibrating or training the instrument with known samples containing the same chemical. The characteristics determined by this method are then used to classify and identify the chemical in the sample. This method can also be used to quantify the concentration of the chemical in the sample.

This chemometric approach represents a synthesis of chemometric methods with knowledge of the response mechanisms of the sensors. Given knowledge of the sensor materials and their interactions with vapors, it is possible to extract information about those vapors from the array. Once an array has been suitably calibrated on known vapors, the array response to an unknown vapor can be converted to several descriptors of the detected vapor, even if the vapor was not included in the original training.

This method has been fully elaborated and demonstrated via simulations. Details have been published.

RELATED LINKS

» **“A Method for Chemometric Classification of Unknown Vapors from the Responses of an Array of Volume-Transducing Sensors”**

J.W. Grate et al., *Anal. Chem.*, 2001., 73(10), 2239-2244

<http://www.pnl.gov/publications/abstracts.asp?report=87289>



Patents & Intellectual Property

- » Patent #: 6,408,250
- » Patent #: 6,606,567

Technology Portfolio(s)

- » Other
- » Chemical Processing and Catalysis
- » Chemical Sensors

Potential Industry Applications

- » Chemicals
- » Computers & Electronics

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