A GAS SENSOR ARRAY TO IDENTIFY COMPLEX VOC MIXTURES IN BREATH
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OBJECTIVES

- Evaluation of a method using prototype Gas Sensor Arrays (GSA) as a screening for early stage lung cancer by breath analysis
- Creation of a benchmark to enable performance comparison between GSA prototypes and sensor prototypes, using synthetic mixtures of Volatile Organic Compounds (VOC) biomarkers of lung cancer and real human breath.
- Creation of a data treatment and analysis method using pattern recognition techniques

BIOMARKERS

- No consensus on biomarkers - which are the most cited compounds? 181 compounds in total, we need to select the best candidates for testing.
- Special care is needed because of confounding factors:
  - Part of Breath - Ventilation Frequency - Heartbeat Rate - Material Contaminations
  - Age/Gender - Diet - Smoking - Comorbidty - Medication - Histology - Time...
- Small sample pools in most publications call for bigger studies

GAS SAMPLE SYNTHESIS

79% N₂ + 16% O₂ + 5% CO₂
N₂ + 25 ppm methanal and aceton + 1 ppm Acetaldehyde + 0 ppm ethanol + 5 ppm isoprene
N₂ + 460 ppm NH₃
Sæ Teflon FEP (2.4 L) VOCs (g/l) level

GAS SENSOR ARRAY

- Different gas sensors react differently to different mixtures of VOCs (see radar plot opposite)
- Temperature, flow and humidity are critical and must be monitored
- CO₂ measurement for capnography
- Needs to be compared to a method of reference: Gas Chromatography Mass Spectrometry with Thermal Desorption
- Therefore, needs to be benchmarked to enable comparison between versions.
- A high performance array produces data enabling the correct classification of mixture using multivariate analysis

EXPECTED OUTCOME

- Experiments on dynamic gas dilutions and GSA optimisation will constitute a base of knowledge for other projects studying VOCs at low concentrations
- Benchmarking approach to optimisation is portable to other projects using Gas Sensor Arrays
- This PhD Thesis is contributing to the creation of a portable screening device against lung cancer, which could also be used to detect other diseases

Sensing of Atmospheres and Monitoring

BENCHMARKING

- Expose the array to two different mixtures repeatedly. The less the difference between the mixtures, the harder the benchmark becomes
- To stay relevant, populations of lab made mixtures should be as close as possible to real breath in composition and variety
- Real breath samples are collected as well to evaluate the device in small scale field use conditions. The influence of sampling conditions and other influences on the classification should be investigated
- Automated data pretreatment synthesises the GSA’s output
- Principal Component Analysis enables the visualization of the data’s structure (see below)
- Classification performance as a metric of GSA’s capacity to differentiate between cancer and healthy breath
- Various multivariate analysis methods will be tested for classification: k-NN, LDA, Neural Networks, PLS, Random Forest, ADABoost.