Milk supervision

created : 13.12.2006
changed : 14.12.2006
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Introduction

The Electronic Nose PEN was used in order to see if the system is capable to distinguish between different milk qualities. The following samples have been analyzed:

Sample	
Tetra pak	"key sample"
Milk A	
Milk B	
Milk C	

An investigation on this discrimination of the different milk qualities with the PEN-system was carried out in order to determine the optimal conditions for the analysis.

Device

PEN3 is our small, fast and robust identification system for gases and vapours. Single compounds or mixtures of gases can be recognized after a "training" step. With its variety of pattern recognition algorithms the system can be adapted to a broad range of applications.
An electronic nose does not provide any information about the chemical content (species, quantification) of a sample. With a training set (pattern) it is capable of distinguishing quality features for a given problem (discrimination). Or it may be used for discovering deviations between standards and differing samples.

Is it possible to detect smell? NO, but a correlation is possible! When?

- If the main components are also the odorous compounds (e.g. industrial process gases).
- If the odorous compounds correlate with the main compounds (indirect detection).

The basic principle of operation of Sensor-Array-Instruments (so-called "Electronic Nose") is well known by chemists around the world. A Sensor-Array always consists of a combination of chemical sensitive sensors. The signals obtained from these sensors are related to the gas composition currently measured and can be compared with previously stored pattern.

With the built-in pumping system and on-board computer the PEN is capable of performing stand alone measurements. In addition the system is configured to avoid a saturation of the sensors through a system that dilutes the sample gas, which is carried out at the inlet of the device (Automatic Ranging).

As an option it is also possible to preconcentrate the samples. With the Trap and Thermal Desorption Unit (EDU) samples can be enriched and preconditioned for the subsequent sensor array analysis. By this way the detection limit of the electronic nose is reduced to the low ppb concentration range.

Procedure

For a measurement series each sample was filled into five separate vials and sealed with a septum before the analysis. Equilibration of headspace took place at ambient temperature for some minutes. Each vial has been analyzed once at ambient temperature. The different samples have been measured using a sequence of alternating classes.
The samples were repeatedly analyzed with this manual headspace method.

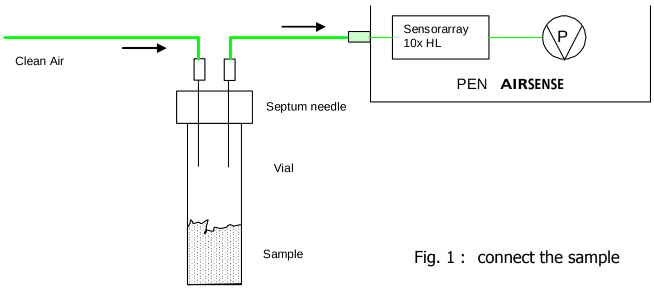


Fig. 1 : connect the sample

The "automatic measurement" procedure provides a simple way to carry out headspace sampling manually. The gas from the headspace of a sample vial is sucked by the measuring instrument for a given sampling period.

Results of the analysis

The following figures display the response of the sensors when exposed to the different samples. One example for each class is shown. The signals derived from the samples are high enough (room temperature) to derive reproducible pattern and to enable statistical evaluation.

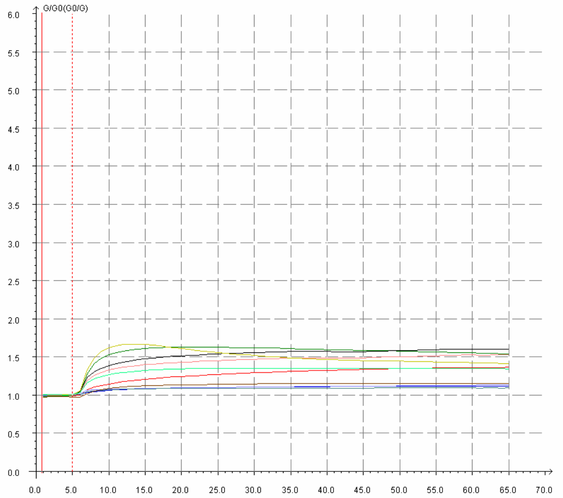


Fig. 2 : Sensor signals "Tetra Pak"

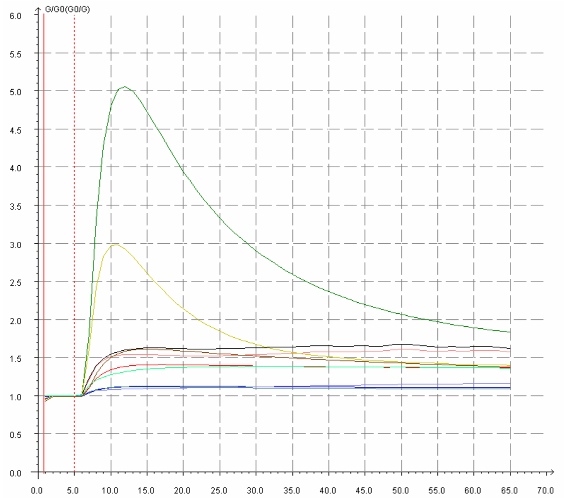


Fig. 3 : Sensor signals from "Milk A"

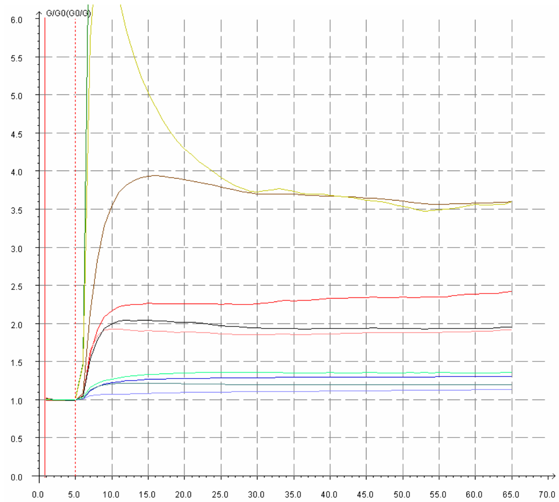


Fig. 4 : Sensor signals from "Milk B"

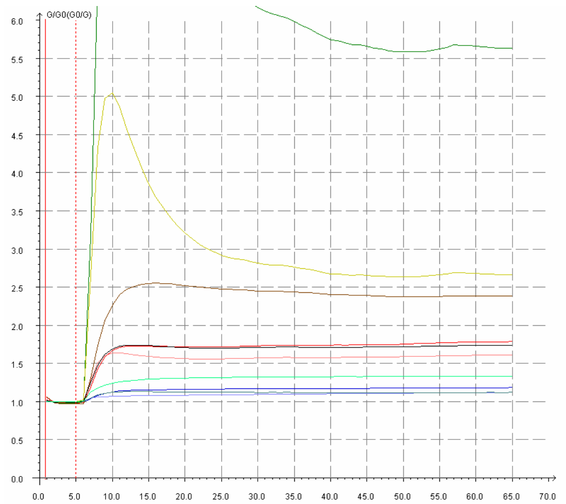


Fig. 5 : Sensor signals from "Milk C"

Drawing all sensor signals from a specific time point (at 60s) the measurement within a polar plot gives a visual idea of a pattern. Differences of measurement signals from "key sample" (Fig. 6) and from a "contaminated sample" (Fig. 7) can be viewed fast and easily by this way.

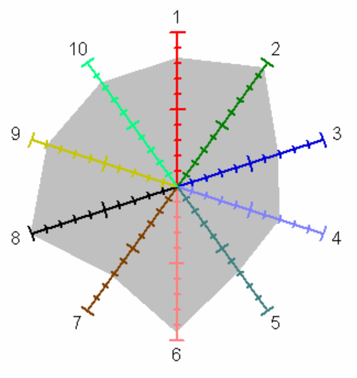


Fig. 6 : Example for pattern Tetra Pak

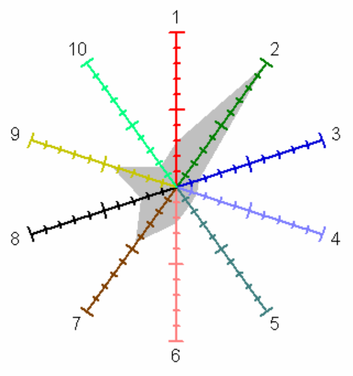
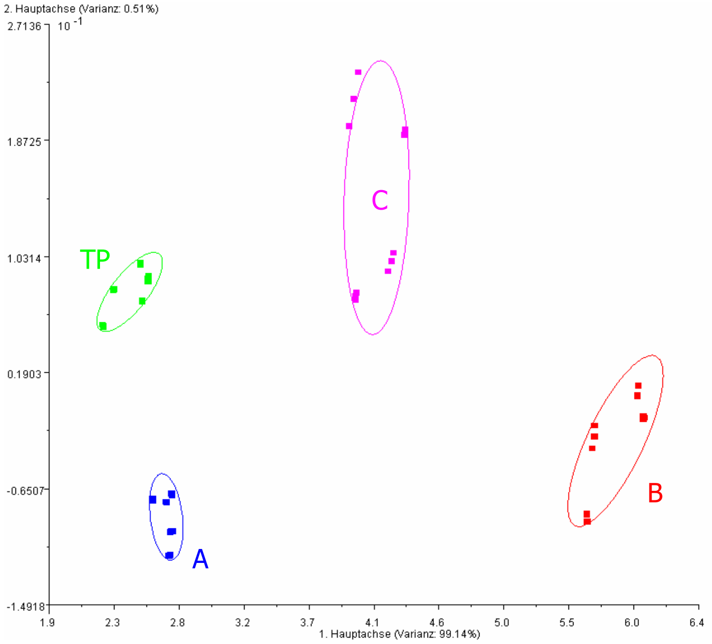


Fig. 7 : Example for pattern "Milk B"

After performing several measurements the training data base (pattern file) was generated. Characteristic data are extracted from measurement files (using the information of all 10 sensors) and combined with the names of the class they belong to.

The pattern is extracted from the measurement files according to a given strategy. Basically, a strategy defines a time point within the measurement file that is used to save the data into the pattern file. This period should contain the most significant sensor signals in order to achieve the best discrimination between classes. A comparison at this period is then possible during production.

The next figure displays the principal-component-analysis (PCA) of the different samples using the information of all 10 sensors.



PCA-Analyse

Normierung : PCA :
Matrix : Correlation-M.
Algorithmus: PCA
Varianz: : 99.647 %
1. Hauptachse: 99.139 %
2. Hauptachse: 0.50876 %
Musterdatei: M:\short-term analysis\39 Spain - Milk\
Discrimination power:

	Tetra Pak	Milk A	Milk B	Milk C
Tetra Pak		0.832	0.992	0.974
Milk A	0.832		0.993	0.976
Milk B	0.992	0.993		0.963
Milk C	0.974	0.976	0.963	

Fig. 8 : PCA – Analysis of samples at room temperature

By using the measurement data (ten dimensions) previously trained, the PCA will then transform the data into 2D coordinates. This is done through the data reduction that extracts the most important information from the database. The results of the transformation can then be displayed within two dimensions.

Training pattern from measurements of similar samples will be located close to each other after transformation. Hence, the graphical output can be used for determining the difference between groups and comparing this difference to the distribution of pattern within one group. The numbers on the right are values of the so-called discriminant power. Two classes are considered to be resolved when the value is higher than 0.5.

The PCA always searches for the view of maximum distribution of all trained data points. It does not care about the class membership.

A further statistical evaluation tool is the linear-discriminant-analysis (LDA). The LDA (Fig. 9) calculates the discriminant functions.

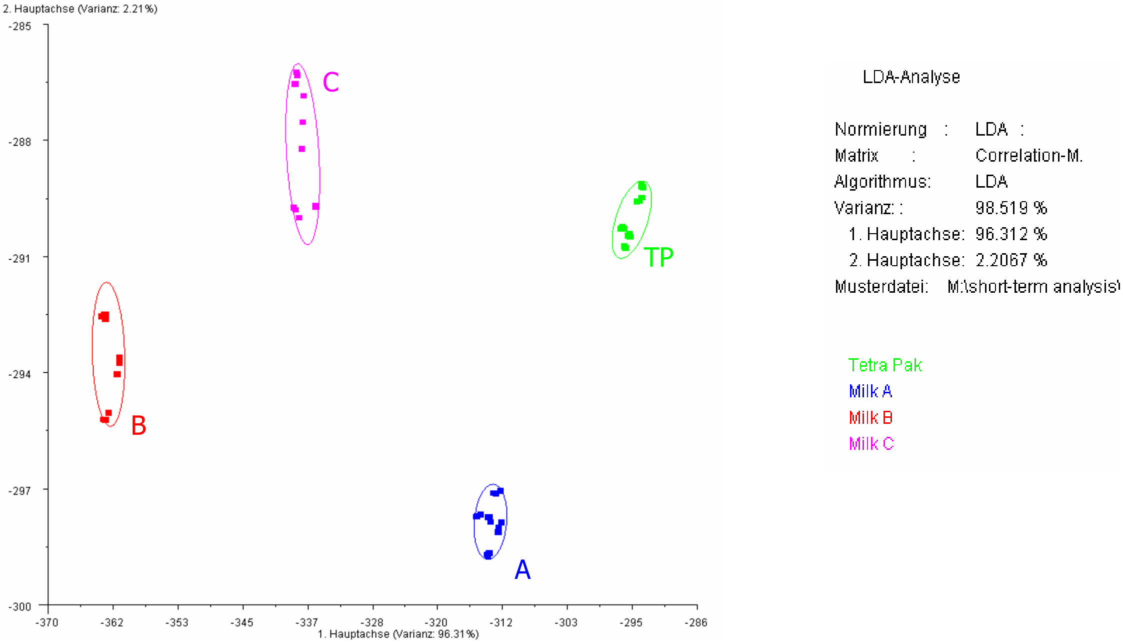


Fig. 9 : LDA – Analysis of samples at room temperature

The functionality is similar the PCA with respect to the following difference: The LDA calculation uses the class information that was given during training. The LDA takes care about the distribution within classes and the distance between them. Therefore, the LDA is capable of displaying a move enhanced resolution. On the other side, the LDA needs a much higher training data set compared to the PCA (at least 60 data points recommended).

The plots show a first axis discrimination of the four given classes. It can be clearly seen that a good (reproducible) discrimination is achieved.

Results

The pattern data base is created by extraction of measurement data within the time range 60 to 62 seconds.

The PCA- and LDA-graphs show the results of the measurements. A discrimination between different milk qualities is achieved easily. This result was obtained without any optimization work for the application (parameters of sampling, training and data evaluation).