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Sensors and Actuators B 101 (2004) 213–223
SENSORS AND ACTUATORS B CHEMICAL
www.elsevier.com/locate/snb

Conference report

2nd Workshop of the Second Network on Artificial Olfactory Sensing (NOSE II)

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Received 27 January 2003; accepted 23 February 2004

Available online 5 May 2004

1. Executive summary

The 2nd Workshop of NOSE II (the Second Network on Artificial Olfactory Sensing) was held in Linköping, Sweden, 18–21 May 2003 and attracted 50 participants from 25 research organisations from 12 different countries. Of these organisations 15 were academic institutions and 10 were companies and end-users (companies, SMEs and research institutes). The main theme of the workshop was 'New concepts for chemical sensing'. A total of 13 key lectures and 10 posters were addressing the following topics:

- Electronic noses—chemical sensors versus analytical instruments
- Electronic tongues
- Current possibilities and pitfalls in data processing
- New concepts for chemical sensing
- Distributed sensor systems

Each session consisted of two or three speakers who introduced the subject, and thereafter plenty of time (30–45 min) for discussion. During each session, experts in the field took notes and later summarised the presentations and discussions. An example of a question discussed is: What do different people mean by the term 'Electronic Nose', or is the term misleading and should be replaced?

During the workshop, there was also a report from the NOSE II Standardisation Working Group, who deals with one of the mostly discussed items at the workshop, namely how can exchange of data and information between scientists in the field be improved? There is a strong need for a standardised data format that satisfies researchers and users and contains all necessary information regarding measurement conditions, and also represents the sensor data in a standardised manner. This would enable benchmarking of different instruments and facilitate exchange of data, e.g. for evaluation of different data processing methods.

There has been no major scientific or technological break-through in the last few years, and the Electronic Nose companies have not become as successful as we may have anticipated a few years ago. We can also see that researchers have to study new fields, e.g. electronics, sampling and data processing, in order to understand and improve the laboratory experiments that previously were made with much less care. Furthermore, several commercial companies have shifted from general-purpose electronic noses to more dedicated sensor systems developed for a particular application. These facts show that the technology has matured, and that the community has learnt from past mistakes. Future directions that were discussed at the workshop include the integration of chemical sensors into large systems, finding new interesting applications, development of novel sensitive materials, and the use of new data processing methods to obtain new functionalities of the sensor systems.

Upcoming events in the NOSE II network

In 2004, NOSE II will conduct three major events for its members and the interested public.

The third short course of the NOSE II network, entitled 'Fundamentals of signal and data processing', is devoted to signal and data processing issues in electronic noses and smart gas sensor arrays. It is scheduled for March in Alpbach (Austria), and is addressed to students, researchers, as well as to members of the industry. The course will cover fundamental concepts with a strong emphasis on the application side (including practical computer exercises).

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0925-4005/$ – see front matter
doi:10.1016/j.snb.2004.02.054

The first workshop in 2004, held at the JRC in Ispra (I), has the main focus on security, food and health, and will be accompanied by a technology demonstration. A second workshop will be a final presentation of the achievements of the NOSE II projects during its 3 years of operation. NOSE II workshops cover actual issues on an advanced level. They are an opportunity to discuss current topics in an audience of experts.

More information on NOSE II and its activities in 2004 is available on the NOSE website: http://www.nose-network.org.

2. Conclusions

Reported by Fredrik Winquist

Udo Weimar, University of Tübingen (ipc), Germany

Chemical sensor systems have developed very far. There is a large knowledge of the various mechanisms, and the field is mature. The name electronic nose may be misleading, however, giving an impression of a system that can do a lot of things. We must be honest, tell what these systems can do and what they not can do. We shall not oversell the concept, something that happened some ten years ago when the technology was young. The validation is thus very important. Chemical sensor system are also not that very much different, either we measure in the gas phase or in the liquid phase. Even if this workshop is dedicated to electronic noses, of course also electronic tongues are important, since these techniques are so related. In some applications, data may be generated by some rather sophisticated and expensive technologies, while in other areas it is not affordable, e.g. the car industry. The data processing people must be aware of what kind or type of data that is generated, an advantage is if they are familiar with the various techniques.

In the workshop, various aspects of the e-nose and e-tongue technology were enlightened and discussed. On Monday, the technology were described and discussed, and on Tuesday the data processing was enlightened. The question was raised what to do with the data. There are many possibilities, both for general improvement of the performance of e-noses and e-tongues, and for drift compensation. In the following discussion, also the question was raised if we really need new sensors, and do we need more data processing techniques. Furthermore, since the technology has a cross-interdisciplinary character, it is necessary to have a good collaboration between people working in the fields of chemistry, physic and data processing. On Tuesday and Wednesday, we also discussed new concepts such as new sensor principles and data processing on distributed sensor system. In this respect, the concept of 'nanospagetti', that is gas sensing based on semiconducting nanobelts appeared to be a very nice concept.

What will we do in the future, and what will we recommend to the EU-commissionaire? A proposition that was raised was the 'pollution network'. We will also have an evolution in the NOSE network. The network must be in all of us—appropriate tools must be used to communicate within the members—and it should be frequent and active.

3. Session reports

3.1. Session 1. Electronic noses—chemical sensors versus analytical instruments

Reported by Mats Eriksson

Chairman: Anita Lloyd Spetz

Recently it has been possible to buy an electronic nose based on a mass spectrometer. Also other analytical instruments can be, and are, used as parts of electronic noses. In this session a comparison of analytical instruments and chemical sensors as the gas sensitive part of an electronic nose was made. Also comparisons with human sensory panels are treated. There was also a discussion about the term 'electronic nose'. What is really the definition of the term and is it useful to use the term?

Thierry Zesiger, SMart Nose, Switzerland

"Electronic noses: a quest for the Holy Graal... a reflection about odours, headspace and means to analyse volatile compounds"

The speaker presents the SMart Nose system which is a mass spectrometer based gas analysis system with data evaluation possibilities such as principal component analysis (PCA). The speaker points out the advantages of using a mass spectrometer instead of chemical sensors in an electronic nose. One big advantage is that it is relatively easy to get rid of the humidity problem, which often occurs when using chemical sensors. With a mass spectrometer all detected compounds are ionised and are measured according to their mass/charge ratio (m/e). In principal each m/e is then a discrete sensor with a unique selectivity. Water, for example, is only detected for $m/e = 18$ (and to a small extent also at lower m/e). If now only peaks for $m/e > 18$ are studied there will be no influence from the humidity.

Other molecules that can disturb the measurement with chemical sensors are ethanol ($m/e = 31$ and 46) and CO_2 ($m/e = 44$). Now if the measurement is performed for $m/e > 44$ we get rid of the influence of all these molecules and can start looking at the more subtle response from other molecules. Thus with a mass spectrometer we can tune the selectivity towards the molecules we are interested in.

In general the advantages of a mass spectrometer based system, compared to an electronic nose based on chemical sensors, can be summarised in the following way:

- **Selectivity**: well defined and resolved channels.
- **Dynamic range**: 6–7 magnitudes from highest to lowest signal.
- **Linearity**: response proportional to concentration.

- **Internal standards**: some mass channels (i.e. argon) can be used to normalise measurements and reduce the drift of the instrument.
- **Data transferability**: from one MS-based e-nose to another MS-based e-nose, and from an MS-based e-nose to other MS instruments (i.e. GC-MS).
- **Information about the sample**: we can know what is producing the signal (sometime with the need of complementary measurements).
- **Sensitivity**: under ppb range in the case of simple matrices.
- **Speed**: due to specific design (vacuum, heated transfer line and injector) the baseline recovery is reached in a few seconds.

The speaker admits that there are also certain drawbacks with a mass spectrometer based system compared to an electronic nose based on chemical sensors:

- **Cost**: the price is high; about €100,000.
- **Weight**: the instrument is heavy and not portable.

There is also the general problem to identify a trace compound in a complex mixture.

There was a question after the presentation about how many channels that are typically needed in a certain application. The answer was that 3–20 channels are used depending on the application and that 4–6 channels are often enough.

Patrick Mielle, Institut National de la Recherche Agronomique, France

"Applications of chemical sensors and analytical instruments for aroma"

The presentation started with a few words on human olfaction. The detection limit can be very low, in the order of 1 ng l^{-1}. The detection limit also varies strongly between different compounds at least by 10 orders of magnitude. The detection limit can also differ strongly between individuals, by a factor of 50–1000. The sensitivity is not the same for all concentrations, but rather follows the so-called Steven's slope.

The state of the art in odour detection is, first of all, sensory panels and, secondly, separative analysis with gas chromatography and other methods. There are also 'global methods' (without separation) like mass spectrometers, gas sensors and liquid sensors.

Very seldom a correlation is found between the results of a sensory panel and with instruments. Some reasons for this are that:

- the concentration might be below the detection limit for the instrument but not for the human nose;
- there might be a presence of interferents in high amounts (like humidity, alcohol, CO_2);
- the instrument measurement is often only semi-quantitative.

A remark about chemical sensors is that the choice of sensor technology is in most cases not the actual problem. It is more important that the sensor cell is carefully designed.

The speaker gave several examples where the odours from different samples were measured both with a sensory panel and with instruments. It is rather seldom that the results from the instruments agree with those from the sensory panel. One lucky example however is barrel toasting where the difference between heated and unheated oak can be detected by both methods. Some unlucky examples with no correlation are the headspace of extra virgin olive oil and off-odours in packaging.

Finally a strategy for making a feasibility study was presented:

- You need a lot of samples!
  - experiments with some extraction-enrichment techniques
- Representativeness test with an external panel
  - choose the technique with less distortion
- GC-olfactometry
  - odour identification
- GC-MS analysis
  - chemical identification of markers
- Selection of the key odorants
  - specifically responsible for aroma or off-odours
- Application to the sensor arrays
  - . . . must work only now!

A question was asked regarding molecules, for example water molecules, that often surround volatiles. This 'water layer' is not detected by most analytical techniques but is important for human smell. The speaker agreed, the matrix is typically stripped off during analysis. Another problem is that the interaction between molecules cannot be detected either. This means that it will not be possible in many cases to correlate analytical measurements with human perception until we know exactly what the human nose smells. Today we cannot make analytical measurements at the same conditions as for human perception. That is why we are not actually doing artificial olfaction, it is something else.

Some questions were asked about sensory panels and panellists:

- How many panellists are there in a panel? The answer is that 50 persons are first screened. Of these persons 12 are chosen who are representative of the consumers.
- What about southern and northern Europeans, do they detect a certain odour differently? The answer was no. They will show a difference in preference, but if they are asked to describe the smell their descriptions will be very similar. In that respect a trained and screened panellist is really an analytical tool.
- Does this mean that the panel should be local for a certain region? There are two kinds of panels, the descriptor panel and the consumer panel. The descriptor panel is there to describe the odour and is therefore 'universal'. The consumer panel should be representative for the consumers and might therefore be local.

Udo Weimar, University of Tübingen (ipc), Germany

"Added values of chemical sensors in electronic noses"

The market for e-noses has been quite exhagurated in the past. Part of the problem when making market estimates is to define what an electronic nose is. When chemical sensors are to be used some basic requirements and considerations are important:

- The chemical sensors must be useful and good. For example it must be possible to produce several sensor systems (instruments) that give the same results (reproducibility).
- We must get useful and good signals out from them that correlate with the quality/quantity to be predicted.
- Nowadays sensor systems exist where the sensor drift is not a problem anymore. It is possible to do a re-calibration with an external standard after some time in order to solve the drift problem.
- There has been a tendency to underestimate the amount of application development that is needed to solve real life problems.

An example with a study of quality prediction of packaging materials showed that it is possible to predict odour quality with a chemical sensor system and get a good agreement with the prediction by a human sensory panel. The results are however not general, it is important to first check if it is reasonable to solve the specific application with chemical sensors. For all applications we are trying to solve there is a reference method established. This should first be used in order to get some experience in the application.

There has been a considerable lowering of the price in the last 10 years for electronic noses, from about €100,000 in 1993 to about €5–10,000 today. Despite this dramatical drop in price there has not been a sufficient penetration in the market for e-noses. Even if the price continues to drop at the same pace it will take several decades before the price has dropped to the region of €10 or so, where a larger market might be expected. This means that we have to do something different. Actually, a parallel development has already occurred for the last ten years for more application specific sensor systems. Already in 1993 it was possible to buy a small system with a Figaro sensor and a particle filter in a small box for about €10. Today it is possible to produce sensor systems for flap control in a car with much more content for about €15–20. An example was given with such a system produced by Bosch to be put in Mercedes cars. This system contains two chemical sensors, a humidity sensor, temperature control, particle filters, a micro controller, other electronics and a data bus.

So, the 'classical e-noses' (either with chemical sensors or mass spectrometer based) can be used as a development tool but will have a rather limited market. The trend for chemical sensors is probably more in the direction of the consumer market. Here something that might be called an 'application specific sensor system' ('a triple s', Andreas Hierlemann) is more useful and competitive. Some examples of applications can be found in the fields of the automotive market, domestic appliances and gadgets. The speaker suggests that the NOSE network should also adapt to these trends.

In conclusion we should think about where chemical sensors are needed. This is where price, power consumption, size, weight and potential of sensor distribution play an important role.

A question was asked concerning the price of application specific sensor systems produced by Bosch. It has been shown previously that the price of sensor systems is not due to the sensors, the electronics, the packaging etc. but rather for the man months put into sales activity. Is it only the number of devices produced that brings down the cost of the Bosch sensor system? The answer is yes. Firstly, there is actually a market pull for these devices and secondly, these sensor systems are bought in several hundred thousands. A comment from the audience was that there is a big difference between e-noses and the Bosch system. The Bosch system is delivered with a very specific application in mind, with a very precise functionality that it should deliver. E-nose systems are produced for whatever you want to do and they have started with the promise to deliver objective odour analysis. That is probably the reason why the market has not taken off, because they could not deliver that. The initial idea of the electronic nose was to put together some sensors and to use data analysis and by that get an objective measurement for odour. We have learnt by now that this is not possible. Another way of putting it is that the e-nose has a technology in mind but the Bosch system (and other similar systems) has the customer in mind. It is important that the system brings some added value for the customer. If you look at a certain market, there is a price that the consumers are willing to pay for a certain function. The higher the added value is the higher the price of the sensor system can (and will) be.

General discussion

When comparing a mass spectrometer with a chemical sensor, we note first of all that different parameters are measured. With the chemical sensor different physical and chemical parameters (such as adsorption and absorption mechanisms which can be dissociative and/or reactive and dependent on shape, size and charge and so on) associated with molecules are measured while for the mass spectrometer a well-defined physical parameter, the mass of ions (or rather the mass to charge ratio), is measured.

Secondly, for chemical sensors there is a possibility of mass production that can bring down the price. This is more difficult for a mass spectrometer system; even in large volumes it will not be possible to reduce the price very much. There is, however a company in the USA, Mass Sensors, that makes a miniaturised mass spectrometer system. Here, however, some sacrifices have to be made especially concerning selectivity and detection limit. The main application at the moment is leak detection.

There must exist an interesting borderline from a technical point of view where we have to use a mass spectrom-

eter because the application at hand cannot be solved with chemical sensors. Another way of putting it is that the problem at hand must be very well defined before choosing if we should go for a mass spectrometer (or other analytical instrument) or for a chemical sensor system.

We should give a clear definition of the e-nose concept. We have seen now that several techniques can be used as an 'e-nose' (chemical sensors, mass spectrometer and other analytical instruments can probably be used as well). Here are some suggestions/comments that were given:

- An electronic nose should contain a set of non-specific detectors (e.g. chemical sensors). These detectors should interact with all compounds in the mixture.
- An electronic nose gives an odour image (an image which is related to the odour). If we go beyond odours that are sensed by the human sense we should speak about sensor systems. These are systems with an 'increased bandwidth' (including molecules not sensed by humans) and that will give physical–chemical images. The electronic nose is a subset of sensor systems.
- A problem with defining an e-nose as a system that gives an odour image is that we cannot, in general, describe what an odour is. An odour is a huge amount of information that we cannot describe (knowledge is zero), but if we can train a panel of humans on some odours and we calibrate our sensor system with this panel with an e-nose we can get some kind of sensation of an odour. In this way the dimensionality of the information can be reduced and we can get data. If we can learn how to transform information to data with some kind of human calibration we might reach a situation where an electronic nose can give some result related to an odour.
- It is probably important to also include the psychology of smell. It is not just a chemical thing.
- An electronic nose is an instrument that uses the same 'scheme' as the human olfactory system. It does not mean to detect odour. This definition might, however, be confusing for the customer.
- One problem is that the scientific community has oversold the expression from the beginning. From that point of view we should admit that there do not exist e-noses today. We have analytical instruments and application specific sensor systems and data analysis. What we can do today is chemical images but not odour images.
- E-nose does not define a technology, it is a definition of an application. It is a definition of something you want to use to objectively measure odours. Odour in the sense as it is defined in human perception.
- With a sniff you either detect or do not detect an odour. How do we describe the smell? We say that it smells like something, i.e. we compare with previous experience. We do not do chemical analysis.
- One idea could be to define, e.g. 12 basic smells and to train an instrument on these smells. This would be in analogy with the human eye where the artificial eye uses only three basic colours. The problem is that 'basic smells' do not exist.

The chairman brought up another question concerning the reputation of the word 'electronic nose'. Is it good or bad? Some comments:

- For mass spectrometer systems it is both positive and negative to call the system an 'electronic nose'. Smart Nose is intended as a help for sensory panels and as an easy-to-use instrument. The analogy to the human nose is simply that instead of putting the headspace of a sample into the human nose it is put into an analytical instrument.
- The expectations that go with the term 'electronic nose' are typically too high compared to what you get.
- For a company the term 'electronic nose' in the marketing will get the wrong kind of people running to you. People that want you to solve problems that cannot be solved with any other technique. But this is not the kind of applications where a company can make a living. The term is, however, very good to attract investors.
- A problem with the term 'electronic nose' is that it leads in the wrong direction, to a fuzzy corner. If this is the case nobody will be interested anymore. What we need is the interest from SMEs and large companies and therefore the term 'electronic nose' should be avoided.

Finally the chairman asked what is most important for the future. Some comments:

- To get reference instruments and improved sampling systems. Also to find out how to get good correlations between human olfaction and e-noses. This is especially intriguing since, for the last 30 years, it has not been possible to find such correlation even with analytical instruments.
- The purpose of the NOSE network is to bring together all experts on the different aspects of chemical sensing and to have an exchange of ideas. Then someone can identify a certain problem and put together the best combination of all these aspects. There is, however, an optimisation step for all different aspects.
- We can also think about combining gas sensors and liquid sensors.

3.2. Session 2. Electronic tongues

Reported by Tina Krantz-Rülcker

Chairman: Ingemar Lundström

Alisa Rudnitskaya, St. Petersburg University, Russia

"Electronic tongues with emphasis on potentiometric devices"

A potentiometric electronic tongue was presented where a number of ion selective electrodes constitute the sensor array. She discussed the advantages and drawbacks in general of potentiometric chemical sensors. The main advantages presented were; that there is a wide range of available sens-

ing materials and sensors, wide variations in sensor properties, that it is possible to use different configuration (static or flow) and size (bulk or micro), that the technique is simple and easy to use and also to apply for automatic analysis and can be made cheap. The drawbacks presented were that there is an insufficient selectivity of many sensors and that the available number of sensors is far smaller than the variety of analytes. A definition of the term electronic tongue was given; "an analytical instrument comprising an array of non-specific, poorly selective, chemical sensors with partial specificity (cross-sensitivity) to different compounds in a solution, and an appropriate chemometric tool for the data processing". Types of analyses that are possible to perform with the potentiometric electronic tongue are classification and discrimination, qualitative analysis of multiple components simultaneously, process control and taste assess and correlation to human perception. Suggested application fields where the instrument can be used were for food products, medical analysis (dialyses solution, urine, pharmaceuticals), environmental analyses, and in industrial processes.

Examples of results from classification of mastitic and healthy milk, quantification of heavy metals in water, prediction of components in tomato juice, monitoring of cheese fermentation and measurement of bitter taste in drugs were presented.

Concluding questions that were raised by the speaker were:

- Can we claim that an electronic tongue would really sense taste of a product?
- The output of an electronic tongue is correlated to taste and flavour and even aroma and colour attributes of products. Can we name such a system electronic tongue?
- Should we use biological analogies comparing and combining electronic tongue and electronic nose?

The questions to the speaker dealt with the possibility to really measure bitter taste and possible drift problems associated with the instrument. The answer to the first part of the question was that although you are only measuring some substances in the sample it was still possible to separate between different degrees of bitter taste. Regarding drift problems it is very much related to the measuring media. It can be overcome by using flow injection analyses (FIA-systems) or more simply by washing procedures of the electrodes.

Fredrik Winquist, Linköping University, Sweden

"A voltammetric electronic tongue compared to other techniques"

The speaker presented an electronic tongue based on voltammetry and made some comparisons with electronic tongues based on other techniques. The voltammetric electronic tongue presented consist of a number (usually between 4 and 6) of electrodes, a reference electrode and an auxiliary stainless steel electrode to obtain the signals, which are chemometrically processed. The speaker motivated the development of an electronic tongue by the arguments that the combination of different senses is interesting and most probably will bring more information about a sample, and that many processes are best measured in solutions. The advantages that appear to be offered by amperometry are that the technique is robust, simple and that the measurement techniques can be varied (electrode material, applied potentials, pulse techniques, stripping techniques, etc.). It was claimed that it is possible to measure many parameters with a voltammetric electronic tongue like redox active species, pH, conductivity, heavy metals (stripping techniques), information on ions (the non-Faradic current) and charged particles.

Results were presented from measurements on water samples from a drinking water production plant with the detection of malfunctioning in some cleaning steps, heavy metal detection, chemical oxygen demand (COD), conductivity, pH, and zeta potential. Comparisons with a taste sensor from Japan showed that both techniques were able to separate between different detergents. Another comparison with the potentiometric electronic tongue presented in the first presentation showed that both these instruments could classify different molds.

Combinations of different techniques were also presented; a hybrid electronic tongue consisting of the voltammetric electronic tongue and measurements of pH, conductivity, Cl^- and CO_2 were used to separate between different fermented milk samples with success. Results from electronic nose- and tongue-measurements were combined and presented, and an artificial sensor head including a vision, auditory, electronic nose and tongue system as well as a chewing resistance meter was also suggested.

One comment after the presentation was that both potentiometric and voltammetric systems have their advantages as well as disadvantages. A question that was raised dealt with fouling of the electrodes. The answer to this question was that this could be a problem and that it is very important to choose applications where it is possible to solve such problems by electrode treatment procedures like mechanical polishing, use of cleaning solutions or electrochemical treatments.

Eric Chanie, AlphaMos, France

"A commercial electronic tongue—technology and applications"

The third and last speaker of the session presented AlphaMos' electronic tongue for measurements in the pharmaceutical industry. The instrument consists of an array of seven cross-selective sensors (ion selective field effect transistors; ISFET) measuring organic as well as inorganic compounds, a software package, an electronic unit for acquisition and autosampler control and a liquid autosampler. The main objective presented for the instrument is to measure the five tastes: saltiness, sourness, sweetness, bitterness and umami. Stated advantages of the technique were that

it allows testing toxic samples (without FDA approval), almost no sample preparation, can be trained like sensory panels in terms of attributes or quality, and does not fatigue compared to the human tongue (particularly for bitterness measurement). It was stressed that one of the most important advantage was to taste toxic compounds with the instrument and that the detection limit in some cases is even below the human threshold limits. The main application that was presented was for bitterness measurements including masking and matching (drug versus placebo), and securing the sensory quality at scale-up from research level to production of pharmaceuticals. More general application areas that were mentioned were for quantitative measurements, characterisation of flavours and quality aspects of food products.

Different results from measurements of bitterness were presented. The correlation between 'human taste score' of bitterness and the α-ASTREE instrument (the electronic tongue system) was claimed to be good. Another study presented was measurements on apple juice quality to study the correlation between sensory panel data and electronic nose as well as electronic tongue data. The different products studied were grouped similarly using data from the different techniques.

During the discussion after the presentation the reproducibility of the sensor system was claimed to be good and stated that the sensors have a lifetime between 4 and 6 months due to degradation of the membranes. Measurements on external standards are used to compensate for drift. The company is working hard in the area of sensor stability. Another question dealt with the future market for the electronic tongue compared to the market for the electronic nose. The answer was that they did not know but that they never had the same interest for the electronic nose as they already have for the electronic tongue. Plans of combining electronic tongue and nose was another question to which the answer was that it is one of their objectives in a project but that they today have no plans of commercialising such a combined instrument.

Many questions focused on the possibility to actually measure a universal bitterness taste. The general answer to this question was that the objective is to measure bitterness for certain drugs and that proper validation is very important. Someone stated that in one sense it was not obvious what the sensors actually were measuring, to which the speaker agreed.

General discussion

How far away is the miniaturisation of the different electronic tongues? The answer for the potentiometric electronic tongue system was that it is in principle possible but it is expensive to produce and run. For the voltammetric electronic tongue a miniaturised system has been developed and the interesting thing is that when miniaturising the system the result is not only a smaller system but also a system with different properties (possibility to measure in low conducting media due to spherical diffusion). It was also concluded that a miniaturisation is not always the most optimal solution while in other situations is it a crucial fact to make it possible to measure and also produce the devices at a reasonable cost.

Since the aim of the workshop was 'New concepts for chemical sensing' it was also discussed if there are other technologies that can be used for liquid sensing. Suggestions that were mentioned were to use surface acoustic wave devices, modifications of the electrode surfaces, the use of lectins, and scanning pulse reflectometry. However, it was commented that an electronic tongue should per definition be based on non-specific sensors with poor selectivity. Although the stability of the sensor layers, molecules, etc. must be improved. It was also stressed that the data evaluation could be improved and that it was very important that people working with systems generating thousands of data per each measurement are open-minded and take help from experts in the field of multivariate data analysis and signal processing.

Another general conclusion that can be drawn from the discussion is that neither the electronic nose nor electronic tongue resembles their biological counter parts. Taste of food is for example a combination of smell and the five different tastes. To be able to try to mimic and predict tastes, a combination of the instruments would therefore be necessary. A final conclusion from the discussion is that the work should focus on developing application specific sensor systems instead of trying to mimic the biological nose and taste system in a general way.

3.3. Session 3. Current possibilities and pitfalls in data processing

Reported by Tom Artursson

Chairman: Martin Holmberg

Jan Mitrovics, AppliedSensor, Germany

"Hands-on improvements using data processing in electronic noses"

The speaker gave a practical view of PCA and LDA and compared the two methods. Another very interesting subject he came across was how to improve the robustness of the models. The very first thing to do is to find the error sources, from which the error comes; is it from the sample, the sampling system or the sensor itself? If the error is unknown it is hard or impossible to pre-treat the data in a way that really would improve the robustness. On the other hand, if the error sources are known the data preprocessing could be directed and the error itself could be reduced. He gave an example of how the temperature dependency of QMB sensors could be reduced with the help of normalisation.

Ricardo Guiterrez-Osuna, Texas A&M University, USA

"Signal processing methods for drift compensation"

The speaker gave a thorough presentation of different methods for drift counteraction, and possible reasons for

drift were discussed. The drift reduction methods try to compensate for the changes in sensor performance using mathematical models, thus maintaining the gas identification capability of the electronic nose. The different drift counteraction methods were divided into two classes, univariate and multivariate drift counteraction. In the class univariate frequency analysis, baseline correction, differential measurements, and multiplicative correction were discussed. In the multivariate class adaptive clustering, system identification, non-linear regression, component correction, and deflation were discussed. From each method an example was given.

General discussion

In the discussion afterwards, the question 'what is the most common problem in data analysis' was raised. Two subjects were discussed according to this questions, drift and miss of information. Since drift already was discussed by the second speaker, this discussion was quite short. The other problem, missing of information, is very serious since a lot of data analysis problems could be solved if more information was available. This highlights the importance of a close collaboration between the sensor scientists and data analysis community. Another topic that was discussed was the importance of validation of the models used to extract information from the sensor data. A common understanding was that there has been an improvement in this area if we look into the history of the electronic nose, but we could still make improvements in this area.

3.4. Session 4. New concepts for chemical sensing

Reported by Anita Lloyd Spetz

Chairman: Ingemar Lundström

In the session new concepts for chemical sensing was presented, nanobelts as potentially both sensitive and stable sensor material, e.g. phatolcyanines and conducting polymers as electrode material for electronic tongues, theoretical modelling of basic sensor parameters and the use of the computer screen as an analytical tool in, e.g. medical diagnosis.

Giorgio Sberveglieri, Brescia University, Italy

"Gas sensing based on semiconducting nanobelts: a new breakthrough"

The resistivity changes in SnO_2 films introduced when switching the ambient is commonly used for gas sensing. The polycrystalline SnO_2 material, which is normally used, suffers from drift due to grain growth. Single crystals, on the other hand, suffer from low sensitivity due to low surface area.

A method to prepare SnO_2 single crystal nanobelts was presented. In a furnace SnO_2 powder is thermally evaporated and transported by an argon flow to a substrate with interdigital electrodes, onto which the nanobelts are deposited. The surface area is larger for the belt structure, which increases the sensitivity even though this is single crystalline material, which in turn increases the stability. The nanobelts are stable up to 800 °C and up to 2 mm long belts are achieved. Modelling of the depletion area in three types of nanostructures was shown. Examples of the gas-response were given and SEM pictures of nanobelts shown. To increase sensitivity even further catalysts will be included in the nanobelt material in the future, and new binary and ternary oxides will be used to produce nanobelt materials.

There were several questions after the presentation:

It was pointed out that in SnO_2 sensor material normally the contact points between the grains are active in the gas sensing process. In the nanobelt material there are very few contact points. It was discussed whether this is detrimental for the gas-sensitivity.

What about the conductivity in one belt? Could it be used to understand the change in the sensitivity as compared to polycrystalline SnO_2 material? Sberveglieri thinks the response time might increase for a single nanobelt used, e.g. in a transistor.

Single crystals have low catalytic activity, which should be a drawback here. Well, the low catalytic activity is due to a low surface area, which is improved by the belt structure.

Are the nanobelt films easy to handle or brittle and is it possible to stretch a film to align the belts? The films stick very well to the surface of the IDTs, which is part of the reason why this kind of investigations are not yet performed in this very new research area.

Maria Luz Rodríguez-Méndez, University of Valladolid, Spain

"Novel voltammetric sensors based on phtalocyanines and conducting polymers for the evaluation of taste"

Metallic voltammetric electrodes can be used as the sensing units of an electronic tongue. The group at the University of Valladolid has proposed a different approach that consists in the development of voltammetric electrodes modified with a range of materials with different electroactive properties that would allow preparing nonselective sensors endowed with sufficient cross-selectivities. Phtalocyanines or conducting polymers (CP) have been used as electrode materials.

In the case of phthalocyanines, electrodes are prepared using carbon paste electrode technique (CPE) or by depositing films (by the Langmuir–Blodgett films technology or ultra high vacuum evaporation) onto conducting substrates like indium tin oxide (ITO). A large variety of electrodes may be processed from different derivatives of phthalocyanines with different central metal atoms. CPE showed the best long-term stability.

The conducting polymers were deposited by electropolymerisation onto a platinum wire. The electrochemical properties of the sensors strongly depend upon the synthesis conditions allowing a simple modification of the sensor response. Several polymers have been tested and polypyrrole

Table 1
Peak potentials of $LnPc_2$ LB films immersed in 0.1 mol l^{-1} KCl

	Peak II (V)			Peak I (V)		
	Cathodic	Anodic	$E_{1/2}$	Cathodic	Anodic	$E_{1/2}$
$EuPc_2$	−0.3	0.3	0.0	0.78	0.91	0.84
$GdPc_2$	−0.26	0.18	−0.04	0.79	0.88	0.83
$LuPc_2$	−0.25	0.1	−0.07	0.63	0.85	0.74
$PrPc_2{}^t$	−0.22	0.28	−0.03	0.62	0.75	0.68

(Ppy) gave the best result. However, the dopants of the Ppy tend to diffuse out into the solution and redox anions and big doping agents are recommended.

An array of phthalocyanines and CPs were used to discriminate between solutions of foods with bitter taste. The array was also tested for the response to red wines. For cleaning of electrodes KCl cycling can be used in between measurements.

Questions raised after the presentation:

- Is there anything to gain from increasing the voltage?
  In the case of phthalocyanines, the voltage range can be as wide as the window of the solvent. Nevertheless, in the case of conducting polymers, voltages beyond 0.6 V disturb the behaviour of the electrode, probably because a dedoping process occurs.
- Is the catalytic activity increased by using redox and ionic properties?
  Phthalocyanines have a well-known catalytic activity that can be the reason for the apparition peaks that can be attributed to the oxidation of species such as glucose, which is not ionic.
- How large is the selectivity for different metals in the phthalocyanines?
  The oxidation potentials of the phthalocyanines are affected both by the central atom and by the presence of substituents in the phthalocyanine ring as shown in Table 1.
- What about the lifetime of these sensors when measuring wine?
  The lifetime of the electrodes depends on the solution tested. In the case of simple solutions (NaCl, quinine, etc.), the lifetime can be 2–3 months. Nevertheless, when analysing complex solutions such as wines, a careful use of the electrodes is needed and frequent cleaning steps are required to avoid the poisoning of the electrodes. Even if these precautions are taken, the lifetime is lower than for simple solutions (i.e. 20–30 days).

Boris Snopok, Institute of Semiconductor Physics, Ukraine

"Nonexponential relaxations"

Snopok had a theoretical approach to chemical sensors. The surface can be regarded as a collection of effective areas. Topography slows down the response. Strong absorbers are bulk controlled, while for weak adsorbers the bulk is not disturbed. The Langmuir approach was applied to the adsorption process. Surface motion is a long journey of chaotic motion. The adsorption is controlled by a distribution of rates. Adsorbers were divided into weak adsorbers which are Langmuir like, strong adsorbers which are diffusion like, and those in between which are fractal like. For example different organic materials, like phthalocyanines and pentacene, etc. could be classified as Langmuir like or diffusion like.

For the solid–gas interaction gas molecules may interact with receptor centers on the surface or in the bulk or sorption by the gas molecules in the lattice cavities of the solid may take place. This may lead to changes in the film structure, e.g. swelling. The driving forces are van der Waals forces giving different polarisability, induction forces of electrostatic origin showing up as different dipole moments, hydrogen bonding or donor acceptor bonding by nucleophilic groups. An electronic nose for pharmaceutics and a QCM based e-nose as an artificial sniffer were given as examples. Finally spatially and temporally resolved analyte mapping was proposed in order to model artificial architectures for realisation of nanoscale structures, which have self-adaptability, self-sensing, memory and multiple functionality.

Discussion after the presentation:

It was pointed out that cross-section is important.

It was questioned that the bulk really is involved for strong adsorbers, and that adsorption and absorption should be differentiated. Henrik isotherm or the Langmuir will probably apply. The Langmuir like adsorption has OH group on the surface involved.

Daniel Filippini, Linköping University, Sweden

"Computer screen assisted technique"

The computer screen is used as a light source for a chemical sensor system based on the scanned light pulse technique (SLPT) in for example medical diagnosis for simplicity and reduced cost. A web camera is used for readout. The nanoscale frequencies of the red, blue and green light can be used and expensive parts like chopper and mirrors can be replaced. Software has been developed for the configuration of a certain computer screen, including both SED and SRD screens. The files may be accessed from a web page.

Cell viabilities and response to antibiotics may be studied. For example pigment analysis of aggregation of melatonin in fish-flake cells can be performed by this method. The pigment aggregation is sensitive to poisons and hormones, while the aggregation reflects the presence of these substances.

The use of the computer screen when running SLPT was also demonstrated. In this application also a lock-in amplifier is needed. It was explained during the questioning that every computer screen needs calibration.

General discussion

The chairman listed, "New concepts for application specific chemical sensor systems, ASSS: new materials, new

principles, new theoretical models and new infrastructure".

The four speakers were asked to tell us about the biggest challenge (problem) of their technology Maria Luz Rodríguez-Méndez mentioned reproducibility and poisoning of the taste sensors as the biggest problem Giorgio Sberveglieri needed models to explain the different behaviour of the nanobelts as compared to the polycrystalline SnO_2 material. Questions to answer are for example, why are the cross-sections of the nanobelts rectangular? The growth method as well as the interpretation of the results when using nanobelts as chemical sensors needs modelling. What happens when one parameter is changed?

Daniel Filippini: To use the computer screen and a web camera as your equipment gives constraints to what you can do. The question is how far you can go, what measurements are possible to perform. The audience commented that these are commercial aspects. Fillippini concluded that this is an instrument to be used when there are constraints to the availability of equipment.

Boris Snopok: The sensor surfaces should be carefully defined in order to distinguish problems arising from the sensors and from the transducer.

The discussion now took a more general turn:

The importance of sampling was emphasised. A short course on this topic is soon coming up in the Nose II network.

More specific sensors designed for a certain problem were suggested, but Sberveglieri commented that the electronic nose concept was designed as a solution to that.

It was also suggested that it is important to also spend some time to understand the basic mechanisms of the chemical sensors.

It was commented that we should learn from the nature, use small size and multiply!

Udo Weimar concluded the discussion by reporting about the opinion of the EU commission. They want to know what we will do in the future regarding both new concepts but also academically in terms of training and education of researchers.

3.5. Session 5. Distributed sensor systems

Reported by Fredrik Winquist

Chairman: Udo Weimar

In this session the concept of integrated sensor system was presented. Thus, both general concepts as well as specific applications were dealt with. Could distributed sensor systems be a new concept for electronic noses or electronic tongues?

Martin Holmberg, FOI and Linköping University, Sweden

"Network of co-operating physical sensors"

The starting point for this lecture was that sensor systems produce a lot of data. Sometimes, it is also necessary to distribute sensors over a large area. This includes applications such as for environmental monitoring, surveillance, or traffic control.

When the area is large or the bandwidth is limited it is, however, not possible to send all data to a central point. Thus, information systems have to be designed for data fusion in a distributed and autonomous way.

In the lecture, it was shown how a network of co-operating physical sensors was used for classification and tracking of vehicles. One tool for this is to use an unattended ground sensor network (UGS). This is in principle not a new technique, but is simply based on many small sensor units spread out over a large area that have the possibility to communicate with each other. The new approach is that the sensors can be put into a network using intelligent agents, which are autonomous programs with a simple, but specific task. Use of agents offers many advantages, they can be added and subtracted from the system while it is running without requiring external intervention, they are self-configuring, and consistent with the object oriented paradigm. In a specific application, it was described how a hostile vehicle could be tracked and classified over a large area. Sensors will then be placed over the area of interest for surveillance. Two sensors, communicating with each other, will be sufficient for telling the direction and class of vehicle. The topology of the network is important, in principle it is based on that several sensors are connected with one node. Several nodes communicate with each other. The sensor data obtained the will consist of a signature and a direction. Association of data from different sensors is made autonomously before data fusion. The fusion will result in a position and classification. There are four agent types. There is one track agent for each known target, and when the assigned target is tracked the agent moves through the network and combines sensor data with its current perception of the track. The sensor agent controls activation/deactivation of the sensor, and sends data to the local dispatch agent. The dispatch agent passes sensor data to the right track agent. Finally, the node agent facilitates track agent movements in the network.

In an animation it was shown how a vehicle was followed and the track agents moved to minimise the distance to the vehicle. Different signal characteristics made it possible to distinguish between different types of vehicles.

It was concluded that distributed sensor systems are useful for treatment of rather complicated tasks and that the development in data processing is an important tool for the sensor community.

Fredrik Gustavsson, Linköping University, Sweden

"Signal processing and information fusion for distributed sensors"

In this lecture, more application areas concerning distributed sensor systems were described as well as the mathematics behind.

The principle of sensor fusion was described. It is based on basic principles of spatial and temporal averaging when

all sensors measure the same parameter, which is time invariant. Inference of a parameter is made, measured directly or indirectly using one or many sensors at one or many time instants. For temporal and spatial correlation, a spatial and dynamic model was described. Examples described were based on data from both an electronic tongue and an electronic nose.

In one example, automotive navigation was described. Distributed wheel speed sensors and a gyroscope were used, and sensor fusion with map information was performed. In another example, ship/aircraft tracking was performed using distributed passive radar warning systems. Each radar warner measured only angle, they were non-synchronised, and a dynamic model was needed for the sensor fusion. A cellular phone positioning system was also described. Other examples included car positioning using a map and the wheel speed. The system could work both with and without GPS. The principles of Bayesian filtering were discussed, as well as Kalman versus particle filters. For the electronic tongue, a challenge is to develop a dynamic model for the collected current information due to onset of voltage pulses. In an application of measurements of bacterial growth, a dynamic model was developed, resulting in a very large data reduction. It was concluded that sensor fusion is a versatile tool with many applications. Further, the Bayesian paradigm offers a general framework for sensor fusion and the particle filter is a modern alternative and extension to classical Kalman filter approaches.

General discussion

The area of distributed sensor system is a new concept that may be very important for both electronic noses and tongues. One interesting approach is the moving chemical sensor system. The key feature is, however, to find good applications. These may include moving robots to search for gas leaks or people. How many robots should be used? Should it be one complicated or many simple, but communicating?

One approach is the gas distribution surveillance, based on chemical sensor and GPS. In chemical plants, distributed chemical sensors could be very valuable for leak detection. A three dimensional problem may arise, making the system complicated and expensive. Another suggestion was to place chemical sensors in tunnels for the identification of accidents, fire, etc. Using simple camera surveillance appeared to be a better idea. There is a large need for stable sensors. A large distributed system offers the possibility to keep track of pollution in Europe. These systems would be stationary and placed both in cities and industrial areas. The surveillance systems used today are only placed at special localised places to get a general overview, and more sites are needed. A suggestion was raised that the EU commission probably would be positive to the idea. The discussion was concluded with that distributed sensor system is a very useful concept, especially when developing applications for chemical sensors.

Acknowledgements

The local organising committee consisted of Tina Krantz-Rülcker, Pia Blomstedt, Mats Eriksson, Ann-Marie Holm, Martin Holmberg, Ingemar Lundström, Anita Lloyd Spetz and Fredrik Winquist, S-SENCE and Applied Physics, Linköping University, Sweden.

The NOSE II thematic network (EU project, Contract no. IST-2001-32494) is supported by the Information Society Technologies Programme ‘Future & Emerging Technologies (FET)’. The workshop was also sponsored by AppliedSensor AB, Asko Cylinda AB, Otre AB, Tekniska Verken and Vattenfall AB. General information about NOSE II is available on the World Wide Web: http://www.nose-network.org.