Keynote Paper

The process of developing an instrument: the JPL electronic nose

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ABSTRACT

An electronic nose is a sensing array designed to monitor for targeted chemical species or mixtures. From 1995 to 2008, an electronic nose was developed at the Jet Propulsion Laboratory (JPL) to monitor the environment in human occupied spacecraft for the sudden release, such as leaks or spills, of targeted chemical species. The JPL ENose was taken through three generations of device, from basic exploratory research into polymer-carbon composite chemiresistive sensors to a fully operating instrument which was demonstrated on the International Space Station for several months. The Third Generation JPL ENose ran continuously in the U.S. Lab on the International Space Station to monitor for sudden releases of a targeted group of chemical species. It is capable of detecting, identifying and quantifying targeted species in the parts-per-million range in air, and of operating at a range of temperatures, humidities and pressures.

Keywords: electronic nose, spacecraft air quality, chemical sensors, sensing array

1. INTRODUCTION

The ability to monitor the constituents of the breathing air in a closed chamber in which air is recycled is important to the National Aeronautics and Space Administration (NASA) for use in closed environments such as may be found in the crew habitat in spacecraft. For the Space Shuttle, air quality was determined after the fact by collecting samples and analyzing them on the ground in laboratory analytical instruments such as a gas chromatograph-mass spectrometer (GC-MS). The availability of a miniature, portable instrument capable of identifying contaminants in the breathing environment at part-per-million levels would greatly enhance the capability for monitoring the quality of recycled air as well as providing notification of the presence of potentially dangerous substances from spills and leaks. Several experimental instruments have been tested on the International Space Station. These instruments have had various capabilities, and included instruments which take a sample once a day or once an hour, and have used various technologies, including mass spectrometry and infra-red spectroscopy. Among the instruments developed and tested is an electronic nose which was developed at the Jet Propulsion Laboratory (JPL) and Caltech.

An electronic nose is an array of chemical sensors. In the case of the JPL Electronic Nose (ENose), the sensors are conductometric chemical sensors which change resistance when exposed to vapors. The sensors are not specific to any one vapor; it is in the use of an array of sensors, each with a different active sensing surface, that gases and gas mixtures can be identified by the pattern of response of the array. Electronic noses have been discussed by several authors, and may be applied to environmental monitoring and quality control in such wide fields as food processing, and industrial environmental monitoring [1,2]. A baseline of background air is established, and deviations from that baseline are recorded as changes in resistance of the sensors. The pattern of distributed response of the sensors may be deconvoluted, and contaminants identified and quantified by using a software analysis program designed for the task.

The JPL ENose was designed as an event monitor for spacecraft breathing air; it is designed to detect contaminants which are released into the environment, such as from a leak or a spill. The ENose is not intended to be an analytical instrument, nor is it designed to take a snapshot of air quality and report all the constituents of a sample of air. It was designed to fill the gap between an alarm, which does not identify the stimulus, and a full analytical instrument, which does not run continuously. The ENose allows continuous monitoring for 10-30 targeted species which may contaminate air owing to a leak or a spill; it could be used as a trigger to an analytical instrument, and it can be used to track the progress of clean up if a spill has deposited a high concentration of contaminant in the air.

In 1994-1995, NASA funded exploratory research into chemical sensors at Caltech, in the laboratory of Prof. Nathan Lewis. This work focused on proof of the concept that an array of polymer-carbon black composite sensors could be made inexpensively, and that such an array could be used, with appropriate electronics and software, as a continuous monitor for breathing air in an enclosed space. The work at Caltech was successful, and NASA then funded device development work at JPL, while continuing to fund Caltech to study sensing materials. This paper will describe the

Micro- and Nanotechnology Sensors, Systems, and Applications IV, edited by
Thomas George, M. Saif Islam, Achyut Dutta, Proc. of SPIE Vol. 8373, 83730W
 · doi: 10.1117/12.921489

process of development of a fully operational device, the JPL ENose, based on the proof-of-concept work done at Caltech.

The work at JPL was designed to produce a device to be demonstrated in an experiment on the Space Shuttle. This device was called the JPL ENose, later dubbed the "First Generation ENose." It was designed to detect, identify and quantify ten chemical compounds against a breathing air background. Compounds were quantified at the one hour Spacecraft Maximum Allowable Concentration (SMAC), generally on the order of a few tens of parts per million. Data were stored on a flash drive incorporated into the device and analyzed on the ground. There was one major test point at approximately one year; a version of the device was operated in the air return line of an inhabited closed chamber at Johnson Space Center for 49 days; this test was undertaken to demonstrate that an electronic nose could have some utility in monitoring recirculated breathing air. The experimental operation on the Space Shuttle took place in late1998, and the ENose was operated for six days during the flight of STS-95.

As a result of the success of the First Generation ENose, further work was funded at JPL. The goal of the further work was expansion of the analyte set, and development of sensors and software to quantify detected chemical species at lower concentrations. The First Generation ENose was re-packaged in a smaller volume and was designed for real-time operation and data analysis using an outboard computer. Extensive work was done to optimize the active sensing surfaces and the electronics, and a combination of computational and experimental work was undertaken to develop an understanding of the mechanism of sensing. In addition, the response of the sensors and sensing array was studied under varying temperature, humidity and pressure conditions. Work was also done to determine whether the device could be operated under conditions with high levels of contamination. This period of improvement and optimization resulted in a device which could detect, identify and quantify twenty chemical species against various backgrounds. The concentrations targeted were twenty-four hour SMACs. This device was known as the Second Generation ENose. Extensive laboratory testing was done in 2003 – 2004.

Finally, in 2004, the Advanced Environmental Monitoring and Control project of NASA funded JPL to develop a demonstration ENose for a six month experimental period on the International Space Station (ISS). This Third Generation ENose was designed to operate continuously and to provide real time data analysis of responses of the sensing array. The device developed was a self-contained, automated instrument.

2. THREE PHASES OF ENOSE DEVELOPMENT

The ENose development at JPL had three phases or "generations" over a period of about 15 years. These phases brought the device from very early, proof-of-concept of the utility of using polymer-carbon composite sensors in an array to detect contaminants to a fully operational, autonomous device designed to operate on the International Space Station. The final phase of development described in this paper is the demonstration of the technology on board ISS. As of today, NASA has not abandoned the ENose as an air quality monitor, but neither has it decided to use it as an operational instrument.

2.1 FIRST GENERATION ENOSE AND EXPERIMENT ON STS-95

The First Generation ENose developed at JPL was based on work done at Caltech[3,4]. The initial work at JPL involved electronics design to start working toward development of a compact, portable instrument. The initial team consisted of an electronics engineer and a chemist. In this initial work, little work was done to tailor the sensing array to any particular set of analytes; sensing materials which had already been tested at Caltech were used. These sensors were polymer-carbon composite films which were made by drop casting in an organic solvent. Work focused on designing a sensor substrate on which various sensing materials could be deposited and platform on which sensor substrates could be interchanged.

Figure 1 shows a sensor substrate. This substrate was designed as a test substrate on which different formulations of sensing material could be tested. Early versions of the substrate also tested different configurations of the two electrodes used for the resistance measurement[5].

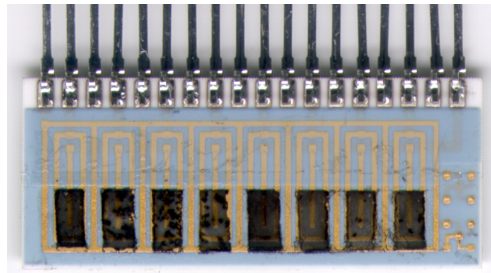

Figure 1. A sensor substrate used in the JPL ENose. Eight polymer-carbon black composite sensors are drop cast onto a masked substrate. Four substrates are used in a complete array.

The electronics designed at this stage of development took advantage of commercially available systems, and an experimental device using a National Instruments DAQPad was built. This device was portable and was controlled by an outboard computer using National Instruments LabView programming.

This device was used to test its operation in the air outflow line of the Early Human Test experiment at Johnson Space Center in 1997[6]. Sensing materials were not optimized in this test and analysis software had not yet been completed so chemical species identification and quantification was available but had not been validated. The purpose of this test was to determine whether such a sensing array could be used to detect anomalous releases of targeted species. This test was successful; the major outcomes were detection of ammonia in the outflow, which was an indicator of a spill from a urine recycling bed and detection of an inrush of humid air from the airlock. The ENose was able to detect these two events. In the case of the leak in the recycling bed, a change in air composition was detected by the ENose about thirty minutes before an odor was reported by one of the test subjects. In the case of the inrush of untreated air, the ENose detected a significant change in humidity and other chemical species, in spite of the test protocols which had used a screen to ensure air integrity.

Further work on the ENose in 1997-1998 took the design of the substrate and electronics and modified them to fit into a flight-approved container. Work in this period also worked to optimize the selection of sensing materials to detect ten target analytes at one-hour SMACs. Sensing materials were selected from those which had been studied in the Lewis lab at Caltech and sixteen were selected for the array using a statistical analysis of sensing material responses. Sensing film processing was optimized to ensure reproducibility from array to array. The DAQPad was replaced by a PIC 16C74A microcontroller and the outboard computer and LabView programming which had been used to operate the early version were replaced with a Hewlett Packard HP200 LX palm top computer using LabWindows programming. The ENose system, including solenoid valves and filters for air comparison, and the electronic circuit are shown in Figure 2.

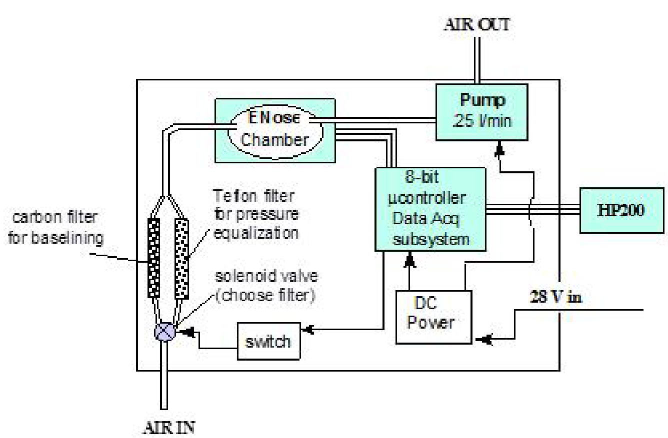

Figure 2. A block diagram of the arrangement of the First Generation JPL ENose. Subsequent version of the JPL ENose had the same basic components and set-up.

The flight version of the First Generation ENose, shown in Figure 3, flew on STS-95 and was operated for six days[7]. Data were collected and stored on the HP200 computer for later analysis. Several excursions in sensor resistance were recorded, and software analysis identified all events which were not operational tests as changes in humidity. Operational tests were identified correctly by the analysis software. Most of those changes correlated in time and magnitude with humidity changes recorded by independent humidity measurements made in the crew cabin. There were no events reported in the shuttle environment that the ENose failed to detect; daily air samples were taken in the vicinity of the operating ENose, and ground analysis at JSC showed no constituents that the ENose should have detected. The ENose experiment was successful, in spite of there being no contamination events to detect, as those events that were detected, operational testing and humidity change, were detected and correlated to log entries and independent sensors. Humidity and operational tests showed that the sensor response was microgravity insensitive[8]. A full description of the First Generation ENose development and flight experiment may be found on the JPL Technical Report Server[9].

Team requirements in Generation 1

To accomplish development of the device for the EHT testing, additional electronics engineers for electronics design and fabrication and an electronics engineer for signal processing design were added to the team. Additional chemists were added to the team as the need for laboratory experiments with sensors developed. To move from the EHT device to the flight-ready experimental device, the members were supplemented by additional chemists and technicians and by a mechanical engineer for packaging assistance. The flight device was assembled by hand in the laboratory.

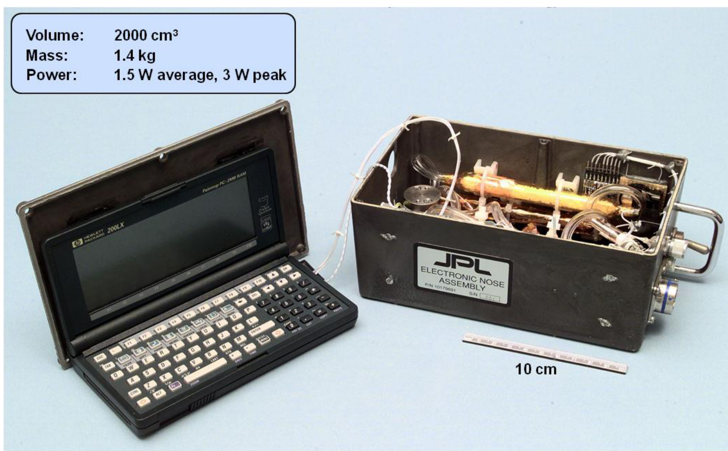

Figure 3. The First Generation JPL ENose flight unit. The palm top computer fit inside the container and was used for device control and data acquisition. This device had a volumeof 2.0 liters, a mass of 1.4 kg and used 1.5 watts average power, 3 watts peak power.

2.2 SECOND GENERATION ENOSE AND GROUND TESTING

Further work with the ENose took into account the limitations of the flight experiment. The experiment was controlled to the extent that daily air samples were taken and daily confirmation of the device's operation was made; however, if an event occurred several hours before the air sample was taken, then the ENose would have been the only detection system. Testing the ENose as an incident monitor required controlled release of target compounds, mixtures of target compounds, and unknowns. This scenario is not a likely one for use in a flight environment, as it could pose a risk to crew health. Thus, the goal of the work on the Second Generation ENose was to improve the packaging and components overall device and to submit it to extensive ground testing in an environment where controlled releases of contaminants could be made and conditions could be varied.

The First Generation ENose, shown in Figure 3, was assembled in a container which was approved for flight. The shape and volume of the ENose were determined by the containers available. Redesign of the packaging focused on design of a more compact container which could accept a battery pack and elimination of separate components such as tubing,

tubing connectors, and a glass chamber cover. The system of four sensor substrates of eight sensors each was retained, and sensor substrates could be changed out easily. Device optimization considerations included the sensing films, methods of data acquisition, and selection of polymers for films in the sensing array. Sensor substrates had been studied in the First Generation work and were not considered in the Second Generation work.

The Second Generation ENose packaging design was subcontracted to Swales Aerospace. The ENose chassis was designed to be made from a block of aluminum which would then be hard anodized for chemical resistance. The design included all the components found in the First Generation ENose; airways were machined into the chassis in place of tubing used in the First Generation, and filter materials, pump and valve were placed integrally into the design. The Second Generation ENose is shown in Figure 4.

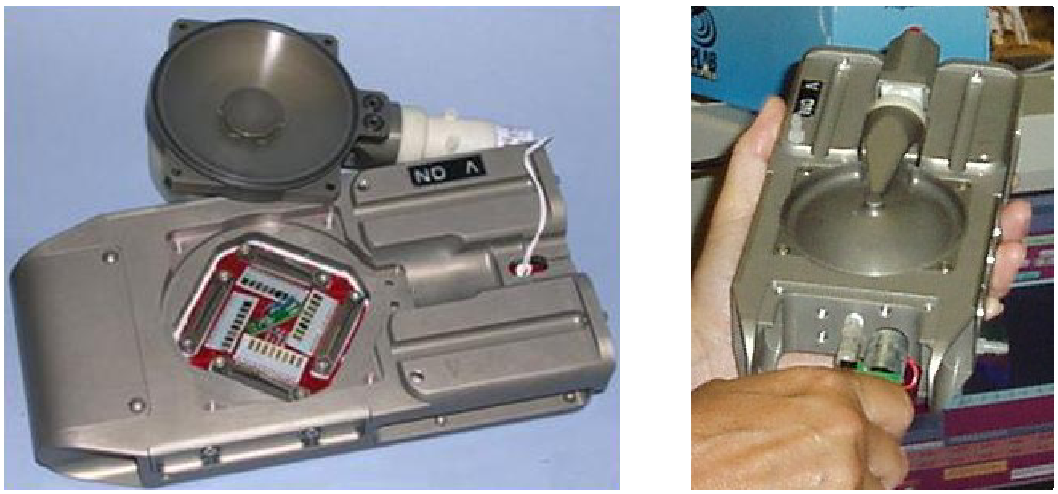

Figure 4. The Second Generation ENose. The ENose is operated by an outboard computer. Power may be provided by a battery pack or line current. This device has a volume of 750 cm^3, a mass of 800 g and used 1.5 watts average power, 3 watts peak power.

Sensing film optimization studies had the goals of increasing sensitivity, to push detection to the 24-hour SMAC, generally single parts-per-million, and to increase the analyte set from ten to twenty-four chemical species. The first pass at increasing sensitivity focused on decreasing noise in the response. Studies with this goal included investigation of the sensor films and of measurement methods. Studies of the films included studies of the polymers used in the films, the solvents, the dissolution and deposition protocols and consideration of several materials as possible replacements for carbon black as the conductive medium in the film. This work also resulted in development of protocols for reproducibility in sensor sets[10,11].

The First Generation ENose used DC measurements to monitor resistance changes in the sensing films; because of the rapid development time for a flight experiment, this approach was taken without study from the Caltech experiments. With more time to consider optimization, AC measurements were considered; such methods might offer insight into changes at the interface of the electrodes and the films and increase the sensitivity.

As the goals of the Second Generation effort included expanding the analyte set, device optimization included development of analytical and computation methods for selecting polymers to use in the array of sensors[12,13]. Previously, polymers were selected by statistical analysis of response of several tens of polymers to target gases. A model of polymer-analyte interaction was developed both to better understand the mechanism of sensing and the role of the conductive medium and to assist in selecting polymers for a specific analyte set.

While alternative conductive materials, such as carbon nanotubes, acetylene black and silver or gold colloids were investigated, and alternative data acquisition methods such as AC measurements, were considered, at the end of the development period of the Second Generation ENose, neither conductive material nor data acquisition method were changed. Carbon black gave the most reliable and reproducible sensors and AC measurements did not offer significant improvement over DC measurements.

The Second Generation ENose was tested extensively in an environmental chamber where humidity and temperature could be controlled in a fairly narrow range (15-50% relative humidity; 20-35 °C). In addition, a vapor delivery system had been set up in the laboratory during First Generation work, and humidity could be controlled over a broad range (0-80% relative humidity) although temperature could not be controlled. Testing could also be done at diminished pressure, to ~500 torr, in the environmental chamber.

At the end of the Second Generation effort, in late 2004, the ENose was capable of detecting, identifying and quantifying 24 chemical species at the 24-hour SMAC, of rejecting unknowns and of deconvoluting mixtures of 2 or 3 target species[14]. It was operated by an outboard computer, such as a laptop, where data acquisition and data analysis could be run, or it was operated by a PDA, where data were acquired and stored for later analysis.

Team requirements in Generation 2

The team for development of the Second Generation ENose was similar to the team at the end of the First Generation. There were several chemists and chemical technicians working on the sensor work, electrical engineers for electronics design and data acquisition code as well as other hardware issues, a mechanical engineer to work with the subcontractor on packaging design and on chassis fabrication, and an electrical/software engineer responsible for data analysis. There was little turnover in core staff between the First and Second Generation efforts.

2.3 THIRD GENERATION ENOSE AND ISS FLIGHT EXPERIMENT

Starting in 2005, JPL was funded to develop a fully operational, autonomous instrument to be flown as a technology demonstration on ISS. This instrument was to be "flight-like" in the sense that the design would be able to be used without significant change to manufacture one or more instruments for flight. The intention was to take the Second Generation ENose as a base and design and build an interface between the ENose and the ISS for power and communication. In addition to development of an interface, the capabilities of the ENose were to be expanded[14].

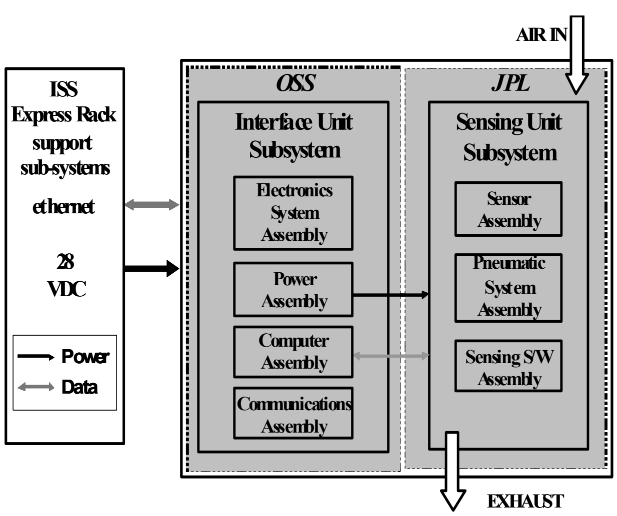

Figure 5. The Third Generation ENose. The block diagram on the left shown the different sunsystems and the interfaces to ISS. The device shown on left was autonomous. It has a volume of 3.6 L, a mass of 3.4 kg and used 8 watts average power and 15 watts peak power. Power was provided by ISS; all other functions are integral to the device.

There were two major areas of development. One area is the design and fabrication of an interface unit which allowed the ENose to be operated through the EXPRESS Rack (EXpedite The PRocessing Of Experiments To Space Station) on the ISS for a long term technology demonstration experiment with continuous monitoring and reporting. In the other area, the capabilities of the sensing platform, the Second Generation ENose, including sensing materials, sensor substrate, and data analysis routines were expanded to include the ability to detect, identify and quantify two inorganic species, mercury and sulfur dioxide, in addition to the Second Generation abilities with organic compounds. The concentrations of the target analytes were based on 24-hour SMACS [16-18]. An additional capability built into the Third Generation ENose is the ability to provide quasi-real time data analysis with read-out on a built in screen. A photograph and a block diagram of the Third Generation ENose are shown in Figure 5.

The ENose was tested in the laboratory before it was launched on STS-126 in November, 2008[19]. The analyte set and quantification targets are shown in Table 1. The JPL ENose was designed to operate in the environment of the US Lab on ISS. It detects targeted analytes at concentrations in the ppm regime at an environmental temperature range of 18 - 30 ^{o}C, relative humidity from 25 - 75% and pressure from 530 to 760 torr. It is designed to run continuously by pulling ambient air over the sensing array. Data analysis was done by the autonomous unit, in quasi-real time, and results were stored for later review. Results of ground testing showed an overall success rate for detection, identification and quantification of all analytes of 87% under nominal temperature and humidity conditions and 83% over all conditions.

Table 1: Analyte List and Target Detection Concentration; mg/m^3 is a pressure independent unit; ppm is for 1 atm.

ANALYTE	QUANT. TARGET (mg/m^3)	QUANT. TARGET (ppm)
Acetone	500	200
Ammonia	3.5	5.0
Dichloromethane	35	10
Ethanol	940	500
Formaldehyde	0.12	0.10
Freon 218	150	20
Mercury	0.080	0.010
Methanol	13	10
2-Propanol	240	100
Sulfur Dioxide	3.0	1.0
Toluene	60	16

Operation on ISS

ENose operated continuously while powered for a total of 4855 hours between December 9, 2008 and July 15, 2009[20]. Figure 6 shows the ENose installed on EXPRESS Rack 2 on ISS in December, 2008. Data were streamed to the operations computer at JPL whenever there was space to ground signal, and full data files were downlinked once a week. Data were streamed through a Graphical User Interface (GUI) designed for the process. Data which were streamed included both Health and Status data for EXPRESS Rack monitoring and sensor data and device health information. The data stream could be read whenever there was Ku Band signal from space to ground.

Data acquired through the ENose GUI were saved on a local computer hard drive. Full files of data and data analysis were downloaded from the ENose to a JPL local computer during weekly command windows, via the Huntsville Operations Support Center (HOSC) at Marshall Space Flight Center; data files downlinked included log files, data files and on-board data analysis. These files were saved on a local computer at JPL for review and analysis and for comparison with onboard data analysis. Although the Third Generation ENose was built with the capability to display the results of real-time analysis on an integral screen, analysis was not shown because operation of the ENose was experimental, and operational decisions were not made based on results from ENose monitoring and analysis.

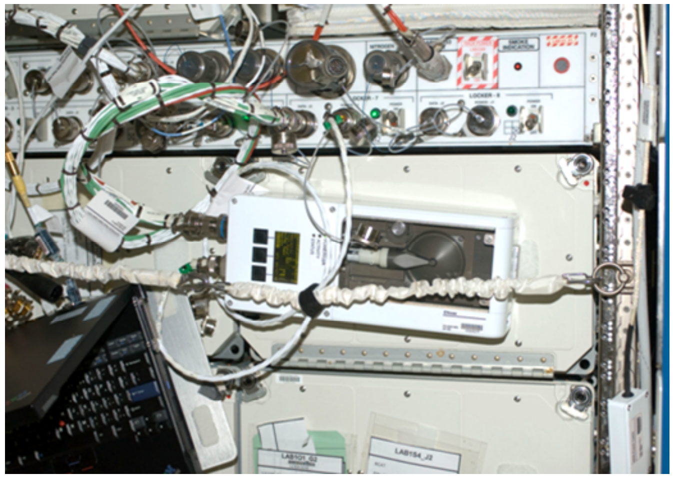

Figure 6. The Third Generation JPL ENose installed on EXPRESS Rack 2 on ISS.

Initial Data From ISS

Initial data sets acquired by the ENose on ISS showed a periodic rise and fall of about 3 percent relative humidity with a period of 144 minutes. The analysis program detected a rise and fall of about 1000 ppm water on a 144 minute period, with little or no time delay.

The periodic rise and fall of humidity was present for the first several days of operation on ISS, then stopped, and humidity and temperature were steady. This rise and fall in humidity was attributed to operation of the Carbon Dioxide Removal Assembly (CDRA), which was under test at the time ENose was activated. The CDRA has a 144 minute half cycle and can expel humidity during the desiccant bed regeneration[21]. Throughout the seven month experimental period, rise and fall of humidity with a 144 minute period correlated with logged times the CDRA was operated.

Events Reported

In normal operation, very few changes in environment which might be considered to be events are reported. The source of these reports is generally crew observation. Samples of air are taken in the US Lab of ISS about once a month. Analysis of those samples lags considerably in time from when they are taken because they must be transported to the ground and analyzed at Johnson Space Center.

Previous work in testing air quality instruments on ISS has included the Volatile Organics Analyzer (VOA) from NASA and the Analysing Interferometer for Ambient Air (ANITA) from the European Space Agency[22]. VOA measurements are taken up to a few times a day, and so provide a snapshot of the presence (or absence) of some forty chemical species, but does not give insight into air constituent changes lasting less than several hours. ANITA measurements are taken more frequently, and the instrument is designed to run continuously. However, measurements are reported about forty minutes apart, and so would not give insight into changes lasting less than one or two hours.

Results from ANITA experiments showed that there was much greater fluctuation in the composition of air in the US Lab than had previously been thought[22]. In particular, the ANITA experiment showed a persistent presence of low-concentration Freon 218 (octafluoropropane) with occasional spikes in concentration. With this knowledge, we expected that we might see changes in Freon 218 concentration in the environment, along with other small organic molecules previously measured in the ISS atmosphere, such as alcohols and formaldehyde.

Over the period of operation, several events were detected. No event was at a hazardous concentration, and most events lasted between 60 and 90 minutes. Table 2 summarizes the species detected, the maximum concentration seen and the number of events.

Table 2: Summary of Events Detected by ENose

Species	No. of Events	Min Con (ppm)	Max Con (ppm)	One Hour SMAC (ppm)
Ethanol	1	450	800	5000
Methanol	24	3	40	200
Formaldehyde	57	0.18	0.22	0.8
Freon 218	19	6	91	11,000
Unknown	22	-	-	-

The most frequently reported events were changes in the water content of the air in the vicinity of ENose. In addition to the humidity variations which correlated well with CDRA operation, there were frequent short-term increases in relative humidity in the mornings and afternoons. These humidity increases are attributed to a crew member exercising, and periods of increase correlate well with time crew members were scheduled to exercise using equipment in the US Lab.

Several short, non-hazardous events were detected, generally lasting one to two hours. This period is consistent with sudden release and rise in concentration of a chemical species followed by a gradual decrease in concentration. Full replacement of the volume of air in the US Lab where ENose was operating takes 11-15 minutes. Four full replacements would take about an hour, which is consistent with the gradual decrease in concentration over a period of about an hour. Four target species and one unknown were detected. It has not been possible to correlate the events with crew or other activities, because we did not have access to enough information about as-performed time lines on ISS to make correlations.

Freon 218 (alternate names: octafluoropropane, perfluoropropane) is a coolant used in the Russian module. Freon 218 is not a toxic species; its 24-hour SMAC is 11,000 ppm, and the maximum concentration seen by ENose is 90 ppm. The ANITA experiment, a European Space Agency Technology Demonstration done in 2008, but not overlapping in time with ENose, was also connected to the EXPRESS Rack in the US Lab. That experiment was not operated continuously, as was ENose, and small molecules such as formaldehyde and methanol were not on their detection target list. However, Freon 218 was on ANITA's target list, and that species was seen frequently as a background trace gas and in "burps" such as might be seen by ENose. ENose would not detect a species always in the background, as it is designed to detect the sudden appearance as in a leak or a spill, but it would detect a species that occasionally occurs as releases. That ANITA detected the unexpected presence of Freon 218 in the US Lab supports the validity of ENose's detection of the same compound.

Post Fight Verification of Detected Species

The ENose was installed on the laboratory bench at the main gas handling system, where training sets were developed. ENose was exposed to three concentrations of each of three of the four species detected on orbit. The exposures were ethanol 450 and 800 ppm, methanol 3 and 10 ppm, formaldehyde 0.21 and 0.25 ppm. These exposures were selected based on the quantities of each of these three analytes detected on orbit, the target detection range, and the quantities which could be delivered without modifying the vapor delivery system. The quantities detected on orbit were ethanol 800 ppm, methanol 3 – 40 ppm with a range of 1 – 10 ppm, and formaldehyde 0.17 to 0.23 ppm with a range of 0.1 – 0.3 ppm.

Each of the analytes delivered was detected, identified and quantified by the vapor delivery system. Ethanol was quantified as 350 and 630 ppm for 400 and 800 ppm delivered. Methanol was quantified as 3 and 8 ppm. Formaldehyde was quantified as 0.19 and 0.23 ppm. In each case, the quantification is accurate to better than +/- 50%, as required.

Detection, identification and quantification of Freon 218 was not verified post flight as the vapor delivery system had been modified and could no longer be used to deliver the appropriate concentrations.

Events of Unknown Chemical Species

Of the 59 unknown events initially reported, 37 were rejected on further analysis. These 37 events were rejected because array response was so small that a fingerprint pattern could not be extracted reliably. Of the remaining 22 unknown events, the array responses were analyzed statistically to determine whether they were similar enough to be considered to be caused by a single stimulus. Of these 22 events, 11 were clearly caused by the same stimulus, 6 were clearly similar to each other and possibly similar to the first 11, and 5 were unrelated to each other or other events. The array responses of the 11 unknown events caused by the same stimulus were analyzed using modeling developed under this program[23,24].

A sensor response model developed at JPL based on Quantitative Structure-Activity Relationships (QSAR) uses a novel molecular descriptor set that developed here; this set combines descriptors of sensing film-analyte interactions, representing sensor response, with a basic analyte descriptor set (e.g. molar refractivity, molecular volume, number of hydrogen bond donor/acceptor sites, dipole, etc.). Statistically validated QSAR models have been developed using Genetic Function Approximations (GFA) for a sensor array for a given training data set.

Using this modeling approach, molecular descriptors for the unknown species were calculated from eight polymer-carbon composite sensor responses. These molecular descriptors were then compared with descriptors for a selection of chemical species. The chemical species which has molecular descriptors closest to the calculated ones is sulfur hexafluoride (SF_6).

A second sensor response model used to determine the identity of the unknown is based on Hansen solubility parameters for the analytes and amorphous polymers. This model was developed by the Molecular Simulations Center at Caltech. Hansen solubility parameters are fitted to measured polymer-carbon sensor responses with physically rooted analytical models. Sensor responses for eight polymer-carbon composite sensors were used to calculate a solubility parameter and molecular volume, and compared with known values for a selection of chemical species. As with the QSAR work, the chemical species with a solubility parameter and molecular volume closest to the values calculated from sensor responses is SF_6.[25]

There are several chemical species that might have parameters similar to those calculated, and so this identification of the unknown as SF_6 is not certain. Calculated parameters do not match those of SF_6 exactly, although they match SF_6 better than any other species considered. In the European Space Agency's ANITA technology demonstration, about 1 ppm SF_6 was found at various times in ISS air[26].

A full report on the development, testing, qualification and flight experiment for the Third Generation ENose may be found on the JPL Technical Report Server[27].

Team requirements in Generation 3

The Third Generation ENose effort was significantly larger than earlier efforts, both because of the requirement for further development of sensing surfaces and of interfacing to ISS, and because of the requirements for Safety and Quality Engineering for operation in ISS. All development associated with the sensing portion of the device was done at JPL. The design and fabrication of the interface unit was subcontracted to Oceaneering, Inc.; members of the Oceaneering team worked closely with electrical and mechanical engineers on the JPL team. The JPL team involved the same group of chemists and electrical engineers as the Second Generation Effort, and was supplemented with systems and quality engineers as well as software engineers.

3. CONCLUSION

Over a period of some 15 years, an electronic nose was developed, fabricated and demonstrated aboard the International Space Station. Work on this device started as exploratory research into the use of polymer-carbon black composite films as the active sensors in a sensing array and was completed with the operation of a fully autonomous device which operated continuously for over 4000 hours. The demonstration period was ended because the designated time for operation was over, not because of any fault or failure in the device. The purpose of this electronic nose is to monitor the breathing air in space habitat for early detection of the release of contaminants into the air. The several events detected during the operational period demonstrate that the device is capable of detecting, identifying and quantifying targeted chemical species.

Over the period of development, a core team of chemists and engineers stayed with the project; this continuity in work force assisted in moving the development forward. At each stage of development, basic and applied research were coupled with engineering and design to optimize a device capable of performing the task set.

ACKNOWLEDGMENTS

The research reported in this paper was carried out at the Jet Propulsion Laboratory, California Institute of Technology under a contract with the National Aeronautics and Space Administration and supported by the Advanced Environmental Monitoring and Control Program, ESMD, NASA.

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