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The ANITA Air Monitoring Programme and Instrumentation – ISS and other Applications

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ABSTRACT

This paper gives a status report on the flight experiment ANITA (Analysing Interferometer for Ambient Air), the development status of the successor unit ANITA II and spin-off activity such as the use of an ANITA-type instrument on a submarine.

The ANITA system represents a precursor for ANITA II, a permanent continuous trace gas monitoring system on the International Space Station (ISS).

The measurement task in a submarine environment is similar to the analysis in the closed environment on the ISS except for the different trace gases present. A proposed test measurement campaign on a submarine in 2006 is outlined in the paper.

The ANITA air analyser can detect and quantify quasi on-line and simultaneously 30 trace gases with sub-ppm detection limits in addition to carbon dioxide and water vapour [4, 10]. This crewed cabin air quality monitor allows the detection and monitoring of trace gas dynamics of a spacecraft atmosphere, providing continuous air monitoring as well as crew warning capability in case of malfunctions.

ANITA will be accommodated in an EXPRESS Rack on the US LAB Destiny. The transportation to ISS is provided by the first flight of the Automated Transfer Vehicle (ATV). Unfortunately, this flight has been delayed until mid 2007. The ANITA team presently works on further improvements in the design and performance of ANITA.

INTRODUCTION

For more then a decade, advanced air monitoring technology for crewed space cabins is under development in Europe. In multiple trade-off and breadboard activities (a cross section of those activities can be derived from [1] - [5], [7] - [10]) and supported by a very successful blind sample testing for NASA [4, 6], FTIR spectrometry was evaluated to be the optimum technology fulfilling the requirements on simultaneous gas detection and continuous analyses of cabin air conditions. The technology maturity has been proven in extensive tests during the breadboard phases and the present ANITA phase.

The optical principle of our system is based on the detection of the different gas molecules' absorption features in the infrared spectra. For the analysis of the measurement results, a sophisticated data analysis SW is applied, implementing a unique optimised evaluation method. With a high time resolution of e.g. five minutes, the ANITA system is able to detect and quantify multiple gases in complex mixtures, even with strongly varying background matrices including water and carbon dioxide.

This paper gives a status overview on the ANITA HW and analysis SW developments and other ongoing team activities like ANITA II pre-developments and, the planning for a real system test on a submarine.

PROGRAMMATICS FOR THE ANITA FLIGHT

The draft agreement between ESA and NASA established early 2004 forms the basis for the ANITA programme. ANITA will be launched with Jules Verne, the first European Automated Transfer Vehicle (ATV1) now planned for mid 2007, and operated in an

EXPRESS rack in the US lab Destiny on the ISS. The data, although experimental, will support the monitoring of trace gases and some major constituents, an analysing process currently failing on the ISS.

Originally designed for a 10-day experiment, ANITA once on the ISS will be operated until end-of-life. The initial plans for support cover a 10-day experiment commissioning test phase followed by an operational phase of 6 months (the extended experiment phase). This extended phase will encompass some additional features for which FTIR technology is attractive, in particular, outlier detection (detection of gases and gas concentrations the system has not been calibrated for), extra sensitive calibration models optimised for the observed gas scenario, and uploading of updated calibration models from ground. To support the handling of any outlier gases, and for HW troubleshooting, an ANITA ground model is introduced, which can be upgraded to flight spare. The extended experiment phase is an excellent opportunity to introduce these features.

ANITA HARDWARE

FLIGHT HARDWARE

As shown in Fig. 1, the ANITA flight HW consists of two mid-deck-locker standard inserts being connected with a set of electrical cables and gas transporting tubes. Further, a laptop computer is required to control ANITA in flight and store the measurement data.

One locker contains the FTIR system and the gas cell, while in the second locker central electronics and a gas sampling unit are accommodated.



Fig. 1 ANITA Flight hardware

The system subcomponents consist of modified and qualified COTS HW with an expectation lifetime beyond 6 months. In the first 10 days commissioning phase the ANITA team tests if the HW is properly functioning and learns about the general system behaviour onboard

ISS., Also it is planned to perform an optimisation process for the measurement parameters and non-local sample tests, which allows analyses on gas samples from different locations on the ISS.

GROUND MODEL SYSTEM

The decision to use ANITA for continuous air analyses of practical importance beyond the 10-day basic experiments led to the need of a system on ground. Thus, during the use of ANITA on the ISS, non-nominal situations and detection of outliers can be simulated on ground, enabling a direct interpretation of the system measurement results and a possibly necessary update of the analysis SW. The ANITA ground model is planned to be ready by May '06.

ISS AIR ANALYSES AND DATA HANDLING

TRACE GAS MONITORING STRATEGY

A major concern during crewed spaceflight is the quality of the cabin atmosphere. In particular, the crew could be endangered by the uncontrolled accumulation of trace gases arising, for example, from off-gassing (from structural materials, electronic equipment, or material used in experiments, etc.), from system failures (leaks, equipment over-heating, fires, etc), or from the crew itself (metabolic products). To ensure a safe atmosphere at all times, these trace gases need to be monitored and controlled below safe limits.

For each trace gas a spacecraft maximum allowable concentration (SMAC) has been defined as a result of medical considerations, previous spaceflight experience, and analogue terrestrial experiences such as in submarines and during saturation diving. SMACs are defined for the short-term (1-24 hours) and for the long-term (7-180 days), depending on accidental releases with manageable effects, or on full protection for healthy crewmembers from adverse effects resulting from continuous exposure to the specific trace gases up to 180 days [11]. To account for cumulative effects of mixtures of contaminants the air quality is considered acceptable when the toxicity index (Tgrp) for each toxicological group of compounds is less than 1, where Tgrp is calculated according Eq. 1:

Tgrp = C1/SMAC1 + C2/SMAC2 + ... + Cn/SMACn (1)

The toxicity index is calculated for each toxicological group. A group is defined according to the target organ and the nature of the toxic response from exposure to the compounds in the group. Depending on the duration of the exposure the target organ and toxic effect can change.

To calculate the toxicity index it is desirable to monitor all possible contaminants in the cabin atmosphere for long-duration missions like the International Space Station (ISS) or Exploration missions. However, this is technically very difficult or even impossible. From extensive analyses of air samples taken from the Space Shuttle and the ISS, it was concluded that monitoring of 25 to 30 compounds would be sufficient to ensure an acceptable atmosphere quality.

	Compound		SMAC [11]					
No	Name	Туре	CUC L	D- 7-		180-	10%	D-limit/
				limits	day	day		10%SMAC(%)
			ppm	ppm	ppm	ppm	ppm	
1	methanol (methyl alcohol)	alcohol	70	0.16	7	7	0.7	23
2	ethanol (ethyl alcohol)	alcohol	30	0.10	1000	1000	100	0.2
			00	0.10	1000	1000	100	0.2
3	2-propanol (isopropanol, isopropyl alcohol)	alcohol	30	0.14	60	60	6	2
4	1-butanol ((n-)butyl alcohol)	alcohol	50	0.3	25	12	1.2	25
5	formaldehyde (methanal) (CH2O)	aldehyde	5	0.051	0.04	0.04	0.004	1275
6	acetaldehyde (ethanal) (CH3CHO)	aldehyde	30	0.13	2	2	0.2	65
7	propionaldehyde (propanal, propylaldehyde) (CH3CH2CHO)	aldehyde	50	0.28	39	*	3.9	0.07
8	butyraldehyde (n-, butanal) (CH3(CH2)2CHO)	aldehyde	0	0.19	40	*	4	0.05
9	toluene (methyl benzene)	aromatic	6	0.24	16	16	1.6	15
10	meta-xylene (meta-dimethyl benzene)	aromatic	15	0.15	50	50	5	3
11	ortho-xylene (ortho-dimethyl benzene)	aromatic	6	0.18	50	50	5	4
12	para-xylene (para-dimethyl benzene)	aromatic	20	0.11	50	50	5	2
13	ethyl benzene	aromatic	20	0.25	30	30	3	8.3
14	ethyl acetate (CH3COOC2H5)	ester	5	0.068	400	*	40	0.2
15	n-butyl acetate (CH3COO(CH2)3CH3, C6H12O2)	ester	4	0.06	39	*	3.9	2
16	dichloro methane (methylene chloride)	hal. hyd.	12	0.088	14	2.8	0.28	31
17	Freon 11 (CCI3F)	hal. hyd.	2	0.007	140	140	14	0.05
18	Freon 12 (CCI2F2)	hal. hyd.	1	0.012	95	95	9.5	0.1
19	Halon 1301 (trifluoro bromo methane) (CF3Br)	hal. hyd.	1.25	0.032	1776	1776	177.6	0.02
20	Freon 113 (CCl2FCClF2, C2Cl3F3)	hal. hyd.	3	0.012	50	50	5	0.2
21	perfluoro propane (octafluoro propane) (C3F8)	hal. hyd.	100	0.028	11000	11000	1100	0.003
22	hexane (n-)	hydroc.	12	0.17	51	*	5.1	3
23	acetone (2-propanone, dimethyl ketone) (CH3COCH3)	ketone	10	0.06	22	22	2.2	3
24	2-butanone (methyl ethyl ketone) (CH3COCH2CH3)	ketone	30	0.071	10	*	1	7
25	hexamethyl cyclo-trisiloxane ([(CH3)2SiO]3 in Si-O ring)	siloxane	2	0.002	102	4.08	0.408	0.5
26	octamethyl cyclo-tetrasiloxane ([(CH3)2SiO]4 in Si-O ring)	siloxane	1.2	0.003	23	1	0.1	3
27	decamethyl cyclo-pentasiloxane ([(CH3)2SiO]5 in Si-O ring)	siloxane	1	0.004	5	1	0.1	4
28	ammonia	misc.	4	0.028	10	10	1	3
29	carbon monoxide	misc.	10	0.026	10	10	1	3
30	methane	back.	500	0.82	5300	5300	530	0.2
31	carbon dioxide	back.	10000	20	7000	7000	700	3
32	water	back.	25028	17				
* Not	defined							

Table 1 – Gas scenario for ANITA: Gas list with calibration upper concentration limit (CUCL) for each compound. Abbreviations and short names for types of compound: aromatic = aromatic hydrocarbon, hal. hyd.= halogenated hydrocarbon, hydroc. = hydrocarbon, misc. = miscellaneous, back. = background gas (always present). Estimated detection limits from the system testing on gas mixtures compared to 10% 180-day (7-day) SMAC. The ratio is given in right-hand column. Values < 100 meet design goals.

The detection limits from the physical gas testing are shown in Table 1. The estimations on the detection limits are based on analyses of gas mixtures where the target gas is *not* present. This approach has several advantages, including independence from the variations in the gas mixing and a common procedure for all trace compounds. The testing of the gas analyses is based on measurements on a set 30 known gas mixtures consisting of three subsets. Each subset contains the three background gases plus four trace gases, all with full concentration variations between the mixtures. For trace gases that are present in one subset of gas mixtures, the calculations are based on the 20 measurements from the other two subsets. For trace gases that are not present in any of the subsets, the calculations are based on 30 measurements. Estimated concentrations of non-present gases reflect the most important disturbances, including interference from other (present) gases, baseline drift and measurement noise. For the background gases, which are present in all gas mixtures, a zero-concentration detection limit cannot be calculated.

In Table 1 the detection limits are compared to the 10%-180-day SMAC values or 7-day SMAC in case the 180day SMAC is not defined. The 10%-SMAC is the design goal for the sensitivity for trace gas monitoring. The ratios are given in '%'; consequently, a value below '100' that indicates the requirement is well met. Formaldehyde, however, can not be detected with the mentioned sensitivity within the given calibration. The approach using a single set of robust calibration models can be refined by introducing local models [9] (see also under definitions at the end of this paper). However, it is presently questionable whether the sensitivity for formaldehyde can be sufficiently increased owing to the high spectral interferences. All other trace gases in the ANITA calibration are well meeting the design goal.

ONBOARD AUTOMATIC ANALYSES

Onboard the ISS a software system will be installed to enable both manual control of the instrument and continuous unattended gas measurement. The software system is fully autonomous and will be started automatically when the power is switched on. After initialisation the system will produce a new air analysis every 5 minutes.

The results from each air analysis include details on, the gas concentrations of the 32 gases in the gas scenario, output from the outlier analyses and evaluation of the system status (see below), and temperature and pressure in the air sample at the time of measurement. All measurement results produced will be stored in an onboard SQL database (Microsoft SQL Server).

For each measurement there will be one foreground spectrum (spectrum measured on the air sample), measured every 5th minute, and one background spectrum measured every 12th hour. The reason why we can allow such infrequent updating of the background spectrum is the stability of the ANITA system, in addition to the effective baseline drift compensation.

Based on the results of every measurement, the software will perform outlier detection. The purpose of the outlier detection is to identify any gases not in the ISS gas scenario, and therefore unknown to the system, and to detect possible gases with too high concentration. Both cases are the result of a situation where the observed gas scenario is out of specification [9]. Results from the outlier detection and the evaluation of system status are also stored in the database. The system

status is classified as normal if no gas is above warning or alarm level, no outlier is detected, and there has been no error or other problem at the time of the current measurement.

Due to the good, but still limited spectral resolution, some gases with narrow spectral lines and high concentrations will give more noticeable non-linear spectral response than others. The system is able to correct for this non-linearity using prior information about the non-linear response of each gas. The corrected gas concentration is stored in the database together with the other concentrations. All gas concentrations stored are referred to 25° C and standard atmospheric pressure 1013.25 hPA [9].

Even though it would be possible, the gas measurements will not be visible to the crew during this first flight of the ANITA system. The reason for this is that the system is not operational, and extensive testing must be performed before the system could be an operational part of the ISS.

ON-GROUND ANALYSES

Each day during the test period, all measurement results will be downlinked to ground for further analyses. An exact replica of the SQL database from the ISS (including everything up to the time of the last downlink) will be built up on ground at SINTEF, based on the data downlinked. The data downlinked will be studied and presented using the ANITA on-ground analysis software. See sample screenshots in figures 2 to 5.

In addition to the results stored in the SQL database, the original measurement spectrum from every half hour and each new background spectrum will be downlinked to ground for further analyses. The planned activities in the ANITA flight experiment include more sensitive analyses with local calibration models [9]. Although these analyses will be initiated manually for ANITA, an operational system could automatically choose between several sets of local models based on the results from the general models.

The downlinking of the measured spectra also opens the possibility for additional analyses on ground, such as more extensive outlier testing or outlier analyses, if required.

Since this is the first in-orbit test of the ANITA system, there will be researchers from the ANITA team acting as "man in the loop", verifying the results before they are presented to ESA and NASA.

The on-ground analysis software can display detailed information about the concentration of each gas in every measurement performed on the ISS (see figures 2 and 4). Since all measurements are stored in the database, the on-ground analysis software can also produce statistics (including plots) of the history of gas concentration changes. It is for instance possible to follow the rise and fall of one or more gas concentrations over time. It is also possible to view the changes of gas concentrations during special events such as a docking to the ISS.

To distinguish between expected gas concentrations at normal operation and high gas concentrations (above the caution or warning level) the software uses colour coding. The user will also be warned about indication of outlier gases (gases not in the ISS gas scenario) by colour coding and additional text explaining the situation (see figures 3 and 5). The system also has the possibility to produce a warning signal if very high levels of gases are detected. (This feature and all other gas information will <u>not</u> be available on the ISS in this experimental phase.)

	Gas Details - Offline Client (GUI)								
formation		Gas	Conc [ppm]	Message		Gas	Conc [ppm]	Message	
	1	methanol	18.979		21	perflouro propane	6.447		
6	2	ethanol	24.09		22	hexane (n-)	0		
)etails]	3	2-propanol	0		23	acetone	0		
iecaiis j	4	1-butanol	0		24	2-butanone	0		
h	5	formaldehyde	0		25	hexamethyl cyclo-trisiloxane	0		
U F Plots	6	acetaldehyde	0		26	octamethyl cyclo-tetrasiloxane	0		
	7	propionaldehyde	0		27	decamethyl cyclo-pentasiloxan	e 0		
*	8	butyraldehyde	0		28	ammonia	0		
💦 rameters	9	toluene	0		29	carbon monoxide	4.01		
	10	meta-xylene	0		30	methane	271.24		
ļ	11	ortho-xylene	0		31	carbon dioxide	7891		
Server	12	para-xylene	0		32	water	3922		
	13	ethyl benzene	0						
	14	ethyl acetate	0						
	15	n-butyl acetate	0						
	16	dichloro methane	0						
	17	Freon 11 (CCI3F)	0						
	18	Freon 12 (CCl2F2)	0						
	19	Halon 1301 (CF3Br)	0						
	20	Freon 113 (CCl2FCClF2)	0						
	Measure	ement temperature (K): 298.15	Measurement pressur	re (hPa): 1013.25					
	Residu	ial Spectrum	St.Dev:	RMS Dev:					

Fig. 2 The figure shows the gas details dialog in the ANITA Analysis Software. The dialog shows the calculated concentrations of all gases in the ISS gas list for one of the gas mixtures in the system testing.

	Gas	Conc [ppm]	Message
1	methanol	38.359	
2	ethanol	178.28	High value indicates outlier
З	2-propanol	32.65	Warning, Concentration limit exceeded
4	1-butanol	0	
5	formaldehyde	0.206	
6	acetaldehyde	5.232	

Fig. 3 The figure is an extract from a dialog like the one in figure 4 showing how outlier detection and a gas level warning could look like. This is a hypothetical example with a synthetic gas mixture.

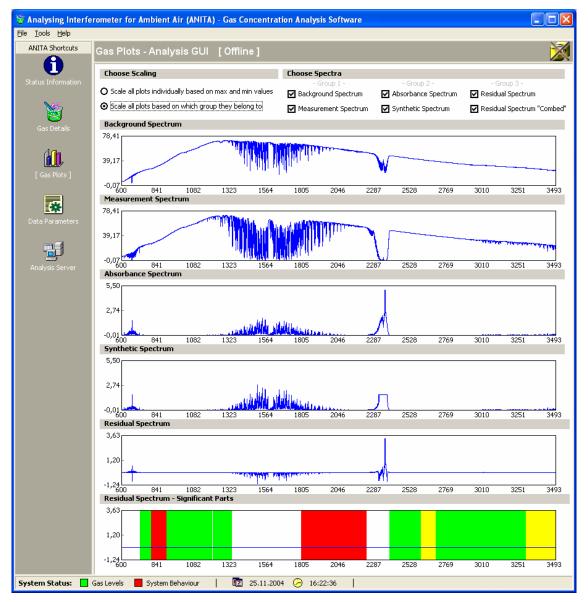


Fig. 4 Gas plot dialog in the ANITA Analysis Software. The plots show the measured background spectrum, the foreground spectrum, the calculated absorbance spectrum, the synthetic spectrum, the residual spectrum, and last the residual spectrum with only the significant parts showing (the other parts are set to zero). In order to see details in the last spectrum, individual scaling can be applied by clicking of the upper left "radio button". Due to the increasing noise and nonlinearities at high absorption levels, the absorbance spectrum and synthetic spectrum are cut off at 5 AU (Absorbance Units). This is a hypothetical example applying a synthetic gas mixture.

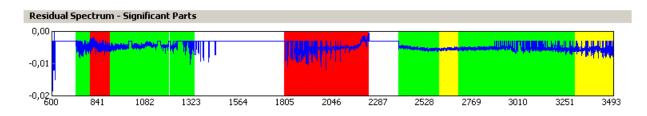


Fig. 5 The figure shows how the significant parts of the residual spectrum may look if there is an outlier gas present in the gas mixture (scaled version of the lower part of Figure 4, applying the "radio button" as described). The green colour coding indicates that everything is normal in that region, the red colour indicates that the standard deviation is too high (above a given threshold) in the region, yellow colour indicates regions approaching the threshold value for abnormal behaviour, and the white regions are ignored. When everything is normal, the residual spectrum should be close to zero (as shown in the green region). The most probable explanation of the high standard deviation is that there is an outlier gas present in the measured air sample. This is a hypothetical example applying a synthetic gas mixture

UPDATING OF ONBOARD ANALYSES

The on-ground analyses of the results and spectra from the ISS could reveal situations not accounted for in the original gas scenario and/or the configuration parameters of the system. One important property of the ANITA Analysis Software is therefore the ability to update the calibration in orbit. It is possible to update the system configuration parameters, and it is also possible to update the system with a totally new calibration. The updating procedure is fully automatic after the necessary files have been uplinked. This means that the process can be controlled completely from ground, and no crew time is necessary.

ANITA II - DEVELOPMENTS TOWARDS A LONGTERM ISS AIR MONITOR

A preliminary design of the ANITA II single mid-deck locker configuration has already been made. It contains a fully operational air monitor inclusive control computer and data storage unit. Selected HW components from the ANITA programme will be optimised leading to improved lifetime and system performance. In the following a summary for the ANITA II system requirements is given

- The ANITA II instrument is foreseen as the second generation FTIR analyser to be permanently installed on the ISS or the CEV (Crew Exploration Vehicle)
- ANITA II ISS will be integrated into one ISS middeck locker (including the data unit)
- ANITA II CEV will be integrated in a system significantly smaller than one ISS middeck locker (including the data unit)
- ANITA II will measure continuously, and the operational lifetime of ANITA II will be at least 5 years
- Non-local sampling will be possible at any time as decided by the end users
- ANITA II will run autonomously without crew interaction (except power on/off, infrequent service activities, and non-local sample collection) and show the results directly to the crew
- Automated TM/TC will be possible including upload of software and model updates
- No consumables will be spent or accumulated, particularly no nitrogen

Thus, the ANITA II development line initially targets on a reasonably 'fast track' towards a one-locker-system for use on ISS. Further development of a smaller and more compact unit – at the moment we assume a size of about half a mid-deck-locker - for use in the exploration programme is foreseen. This small system can therefore possibly be accommodated in the CEV or another crewed Moon/Mars transportation vehicle but could also

be used as sophisticated continuous air monitor in crewed stations on Moon or Mars.



Fig. 6 Compact and sheltered ANITA set-up for the submarine test measurements

PROPOSED TEST OF THE ANITA SYSTEM ON A SUBMARINE

In a closed environment like on a submarine, the crew's health and well-being is strongly dependent on the air conditions. An ANITA-type air analyser with the capability to detect simultaneously and quasi on-line a large number of trace gases can significantly improve the health safety for the crew. The proposed test measurements on a submarine constitute a necessary basis for the generation of a technology spin-off The submarine case is very similar to the application on the ISS, for which ANITA has been developed., A measurement campaign is proposed for mid '06 for one week on a submarine. These measurements form the first step for future air monitoring activities on Dutch, German, British, or French submarines.

The ANITA HW can be applied directly for the task (the corresponding system set-up can be seen in figure 6), while the system will need a new calibration to cover all the gases that are specific to the submarine air environment. Therefore, the ANITA HW will be used with analysis SW tailored to the submarine environment. Owing to the method of calibration, the tailored gas calibration can be performed after the measurements. Time-resolved gas analyses with full quality can then be made post mission on measured spectra that have been stored. – Such post mission calibration and analysis has several important advantages, including quick start-up of

the testing and highly increased confidence that the calibration will really cover the observed air environment (including any surprising gases).

Testing of ANITA in a submarine before the transportation to ISS gives several advantages by consolidating the operational status of the flight experiment as summarised below:

- The operational procedures for ANITA HW and SW, a will be more thoroughly tested in a practical situation resembling the task on the ISS.
- Experience on applying the ANITA system, possibly including use through a third party
- Experience on handling of real measurement data
 - Having measurement noise in the wider sense (including acoustical and mechanical vibrations and traces of compounds outside the gas list)
 - Handling of gas detection significance
 - Handling of outlier detection significance and possible outlier gases
 - Analysing and presenting gas data
 - Experience on making a calibration adapted to an observed gas scenario

CONCLUSION

An advanced air monitoring system has been developed for the ISS and for manned space vehicles for missions beyond LEO. ANITA is a precursor mission on the ISS before the launch of a permanent air monitor ANITA II. Additionally the technology is well suited for advanced air monitoring activities within the exploration programme, in closed environments in general, and for all kinds of multi-gas measurements.

ANITA sensitivity matches very well the design goal, albeit not for all trace gases.

Lessons learned from the ANITA flight experiment in terms of autonomous operation and automatic and reliable data evaluation will be used to define an operational ANITA II system. An optimisation process for different selected subcomponents of the FTIR spectrometer will lead to an ANITA II set-up in one middeck locker and smaller configurations.

The ANITA flight experiment not only allows the demonstration of its full TGM capability, but also provides to the ISS the necessary air quality data (albeit

experimental) currently not available due to the failed VOA (Volatile Organic Analyzer). The original 10-day baseline mission is for this purpose extended as long as ANITA can be kept operational.

The planned system test on a submarine mid '06 forms a very good basis for technology spin-off activities and for testing of the operational procedures designed for later autonomous operation of the ANITA experiment on the ISS.

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DEFINITIONS, ACRONYMS, ABBREVIATIONS

- ANITA: Analysing Interferometer for Ambient Air
- ATV: Automate Transfer Vehicle
- CDR: Critical Design Review
- ESA: European Space Agency
- ERR: Experiment Requirement Review
- **EXPRESS**: EXpedite the PRocessing of Experiments to Space Station (rack for electronic equipment)
- FE: Flight Experiment
- FTIR: Fourier Transform Interferometer/-metry
- HW: Hardware
- **ISS:** International Space Station
- LEO: Low Earth Orbit
- PDR: Preliminary Design Review
- **PLS**: Partial Least Squares (multivariate statistical method)
- SNR: Signal to Noise Ratio
- **SQL**: Structured Query Language (standard computer language for accessing and manipulating databases)
- SW: Software
- TGM: Trace Gas Monitoring

Calibration model: In connection with the ESA TGM system: A vector (set of numbers) to be multiplied with a measured absorption IR spectrum to produce a value for a gas concentration. (One model for each gas compound)

Calibration modelling: The process of producing optimised calibration models, applying advanced simulations and multivariate statistical analyses.

Local (calibration) models: Calibration models applicable to normal or special situations where the gas environment is less difficult than the worst case. Great improvements may be achievable in terms of measurement precision and detection limits. A set of local calibration models can be applied whenever the general, robust set of calibration models show that the gas environment is within the specified limits for the local models. Since the general set of calibration models is always run first, there is no loss in robustness when local models are added, and there is no consequence for the HW.

Outlier: A value or set of values that are abnormal, e.g. out of specification or indicating an error. **Outlier values** or more complex **outlier situations** are discovered through special analyses leading to **outlier detection**, typically leading to a proper **outlier warning**.

Residual spectrum: The remainder of the measured absorption spectrum after the properly scaled reference spectrum for each detected gas compound has been subtracted. In popular terms the residual spectrum represents the "unused" or unexplained part of the measured spectrum.