Progress in ANITA2, the Upcoming High Performance ISS Air Monitor for Continuous In-Orbit Operation

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Following the successful European precursor mission ANITA1 (Analysing Interferometer for Ambient Air) operating on ISS for 11 months in 2007 and 2008, the next generation system ANITA2 is in the design and breadboarding phase. The ANITA1 data have delivered new and partly surprising results on the dynamics of the crewed cabin atmosphere showing the advantages of an optical sensor with high time resolution. The successor instrument ANITA2 is developed to give a system with significant improvements in sensitivity and instrument characteristics. ANITA2 will be calibrated to detect and quantify simultaneously and quasi on-line more than 30 of the most important trace gases in the cabin atmosphere with automatic operation for three to five years on ISS. ANITA2 will be a maintenance-free, reliable, and compact multi-gas air quality monitor.

ANITA2 is like ANITA1 suggested to be an ESA-NASA cooperative programme. It further represents a precursor system for missions e.g. to the Moon and Mars under the manned exploration programme. The following ANITA3 system will be a high performance, maintenance-free measurement unit approaching the size of a shoe box. The paper will report on the newly started ANITA2 development of an instrument breadboard and analysis software pre-developments giving an outlook into the future programmatics. The work described is performed under contract of the European Space Agency ESA.

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Nomenclature

ANITA:	Analysing Interferometer for Ambient Air
BB:	Breadboard
DFB	Distributed Feedback Laser
DLaTGS:	Deuterated L-alanine-doped TriGlycine Sulfate (IR detector)
ESA:	European Space Agency
FE:	Flight Experiment
FM:	Flight Model
FTIR:	Fourier Transform InfraRed spectrometer/-metry
HW:	Hardware
IR:	InfraRed
ISS:	International Space Station
PLS:	Partial Least Squares (multivariate statistical method)
SNR:	Signal to Noise Ratio
SW:	Software
TGM:	Trace Gas Monitoring
IBB:	Integrated Bread Board

I. Introduction

Starting in 1991 the European Space Agency ESA has selected the FTIR (Fourier Transform Infrared) technology to continuously monitor the crewed spacecraft atmosphere quality. Within different study and breadboard activities (compare e.g. [1]through [15]) supported by a very successful blind sample testing for NASA [6, 8] it has been shown, that the requirements on simultaneous gas detection are best fulfilled by an optical analyses method in combination with sophisticated analysis SW (Software).

The system's measurement principle is based on the detection of the IR (infrared) absorption features stemming from the different gas molecules' vibration modes. From the measured IR spectra the gas concentrations are derived via sophisticated analysis SW applying optimised, non-linear data-evaluation methods; (compare especially [3,4,5,11]). The system's capability to measure with a time resolution in the order of minutes allows for the first time to trace the dynamics in the concentrations of trace gases within the ISS atmosphere.

ANITA Background system aspects

The gas mixture which shall be analyzed, is flushed into a gas cell with optical folding mirrors enlarging the optical path length to in total 10 m. Important development steps consisting of an optimization of several HW sub-components have been realized for ANITA (e.g. highly stable opto-mechanical set-up, lightweight high-performance optical modulator, new type of IR source). Important is also the interaction with the specially developed data evaluation SW tuned to the HW performance. This SW is optimized through complex simulations and multivariate statistical analyses, but the runtime SW is simple and fast. Due to additional noise effects during the ANITA mission, supplementary SW activities on the ground model have to be executed to improve the system data evaluation.

In Fig. 1, a sketch of the FTIR spectrometer measurement principle is shown. The modulated infrared radiation from a broadband light source is directed through a gas cell with the air sample (target gases) present. The radiation is then detected and the measured signal applied to the mathematical method of a Fourier transformation. This finally leads to a characteristic spectrum shown in Fig. 2. The wave number range between 600 and 3500 cm^{-1} is used for monitoring of the multiple, gas characteristic absorption features in parallel. The location and details of the absorption bands are used for gas identification and the depth of the absorption for the corresponding quantification.

Owing to the inherent optical compensations in the FTIR measurement principle and the additional SW compensations, the system calibration is in principle permanent. No recalibration is required to handle long-term variations in e.g. the source or the optical throughput of the system.

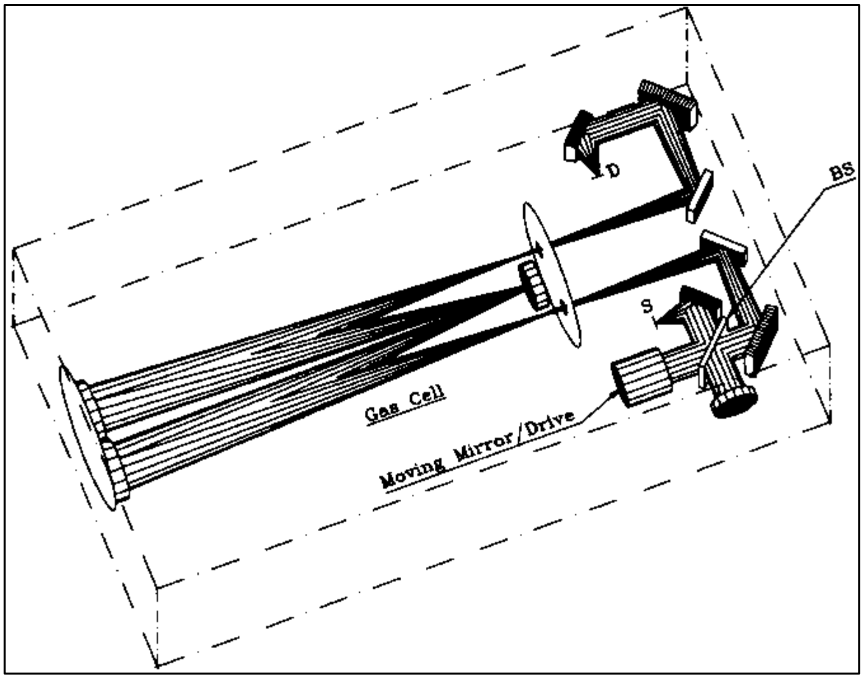

Figure 1. Operation principle of the FTIR measurement system: S light source, BS beam splitter, gas cell & D detector

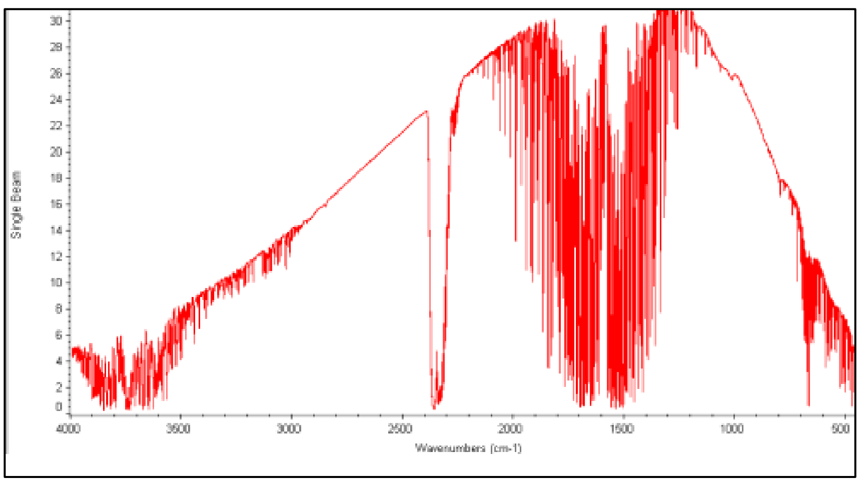

Figure 2. Typical FTIR spectrum detected by ANITA. The embracing curve represents a blackbody with a temperature of 1500 K

II. Background Information on the ANITA1 System

Detailed information on the ANITA1 system can be found in the references[1 – 8]. The system consisted of two specially designed mid-deck locker inserts (standard payload rack inserts) plus support HW. One mid-deck locker contained the FTIR measurement system, the other the electronics and the gas sampling unit. Figure 3 shows the ANITA1 accommodated on the ISS. The measured optical spectra were automatically analysed by sophisticated analysis software to produce a detailed data set on the air quality inside the ISS every six minutes.

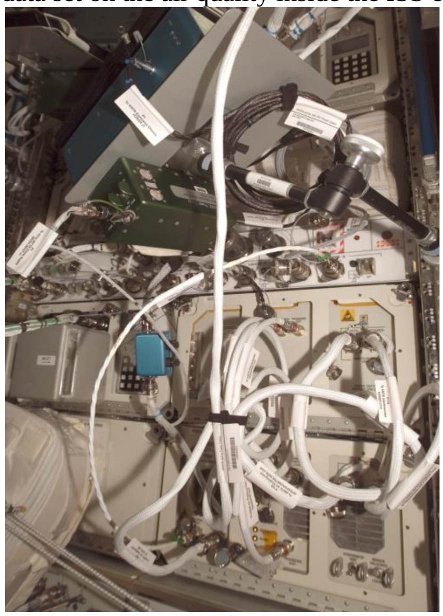

Figure 3. ANITA1 mounted on ISS in the US lab (two mid deck locker inserts, cable sets connecting the two loggers, breakout board, control laptop) (Photo: Courtesy of NASA)

III. ANITA2 System Hardware

In the design of the successor unit ANITA2 the lessons learned from the ANITA1 mission are considered, and stricter requirements on lower mass and volume are applied. One of the main requirements is that the whole instrument shall fit into one mid-deck locker including the control unit (PC). This saves transport of external cables and control parts, and the astronaut's work on the instrument installation is strongly reduced and simplified. To gain more experience an overall new instrument set-up has been designed as breadboard, which allows the accommodation of all newly developed subcomponents in a single mid-deck locker insert.

Table 1 compares the instrument characteristics of ANITA1 and ANITA2, showing the significant improvements in the overall performance and reductions in the system complexity.

System property	**ANITA1**	**ANITA2**
mass	54 kg	27 kg
elements	Two mid-deck locker inserts, connecting gas tubes and data cables, laptop, breakout board	One mid-deck locker insert
power	150 W (peak)	100 W (peak)
sensitivity[1]	good[1,2]	very good, like ANITA1 on-ground[1,2]
response time (full set of data with 33 gases and potential outliers) [3]	3-5 minutes	3-5 minutes

[1] The sensitivity is an individual number for each gas, which also depends heavily on the gas scenario (i.e. all the other gases that may be present). ANITA2 is expected to be typically an order of magnitude more sensitive in operation on the ISS than ANITA1.
[2] ANITA1's actual sensitivity in operation on the ISS cannot be properly quantified, since no test measurement could be performed after installation. The pre-flight test results on sensitivity for ANITA1 are shown in Annex 1. However, since ANITA1 suffered from mechanical micro-vibrations on the ISS, the induced measurement noise reduced ANITA1's sensitivity for gas detection. ANITA2 is expected to exhibit gas sensitivity in operation on the ISS at least matching ANITA1's on-ground performance.
[3] The pre-flight gas list (32 gases) is shown in Appendix 1. The gas sulphur hexafluoride, which ANITA1 unexpectedly detected on the ISS, was included in the calibration after installation.

Table 1: Comparison of ANITA1 and ANITA2 system characteristics

IV. ANITA2 Integrated Breadboard

A. ANITA2 IBB Description

As mentioned above the complete ANITA2 hardware, including the data unit, has to fit into one mid-deck locker insert. During the first ANITA2 design studies a preliminary concept for a single-locker concept has been elaborated. The insert consists of three main compartments: (1) electronics and power module, (2) air sample pumping unit and (3) the optical compartment. The instrument will run under the changing ISS pressure conditiopns avoiding security issues from pressure diffences. The compartments (1) and (2) are actively cooled by fans. The cooling concept is that the optics compartment (3) is indirectly cooled by the fans as well.

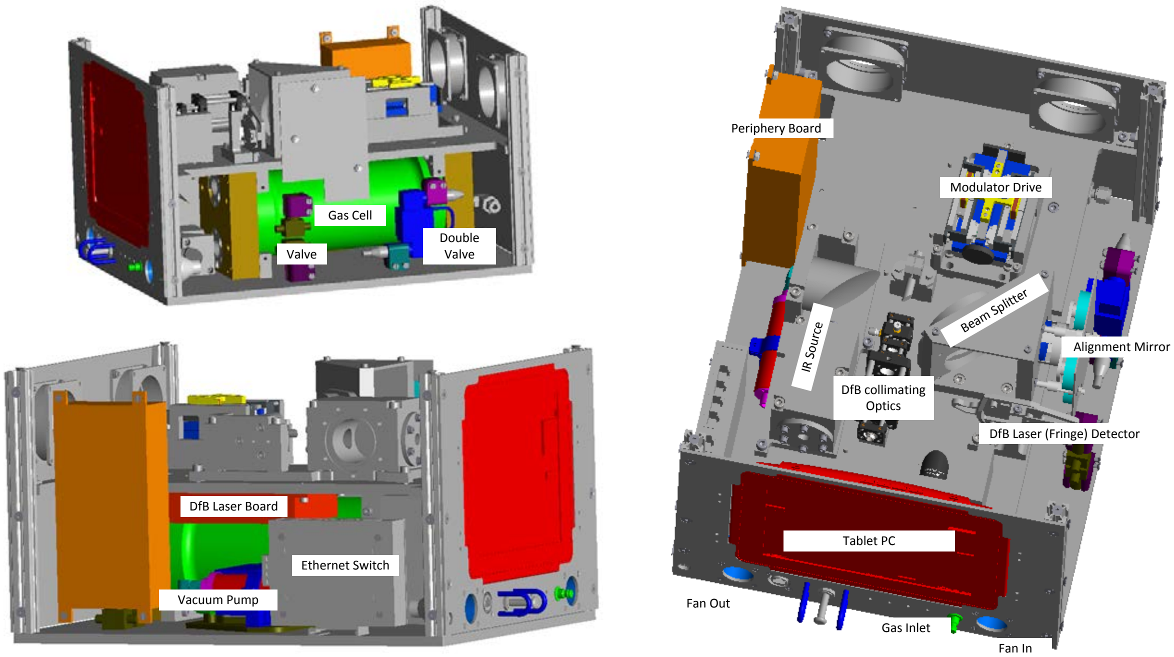

Figure 4: Interior of the Integrated Bread Board of ANITA2.

Figure 4 shows the interior of the ANITA2 IBB hardware. The drawer contains the complete system with its main components:

- Front end Electronics (New Development)
- Modulator Drive (New Development)
- DFB Laser Board (New Development)
- IR Detector Board (New Development)
- ANITA1 FM Gas Cell
- Sealed IR Source
- Air Sampling Unit

B. Front end Electronics (New Development)

The new concept of the front end electronics (FEE) together with the final integrated electronic board is depicted in Figure 5. The FEE controls all subsystems, communicates with the Data Unit (Tablet PC) and acts as power supply. The input power is set to 28V as for the ISS operation.

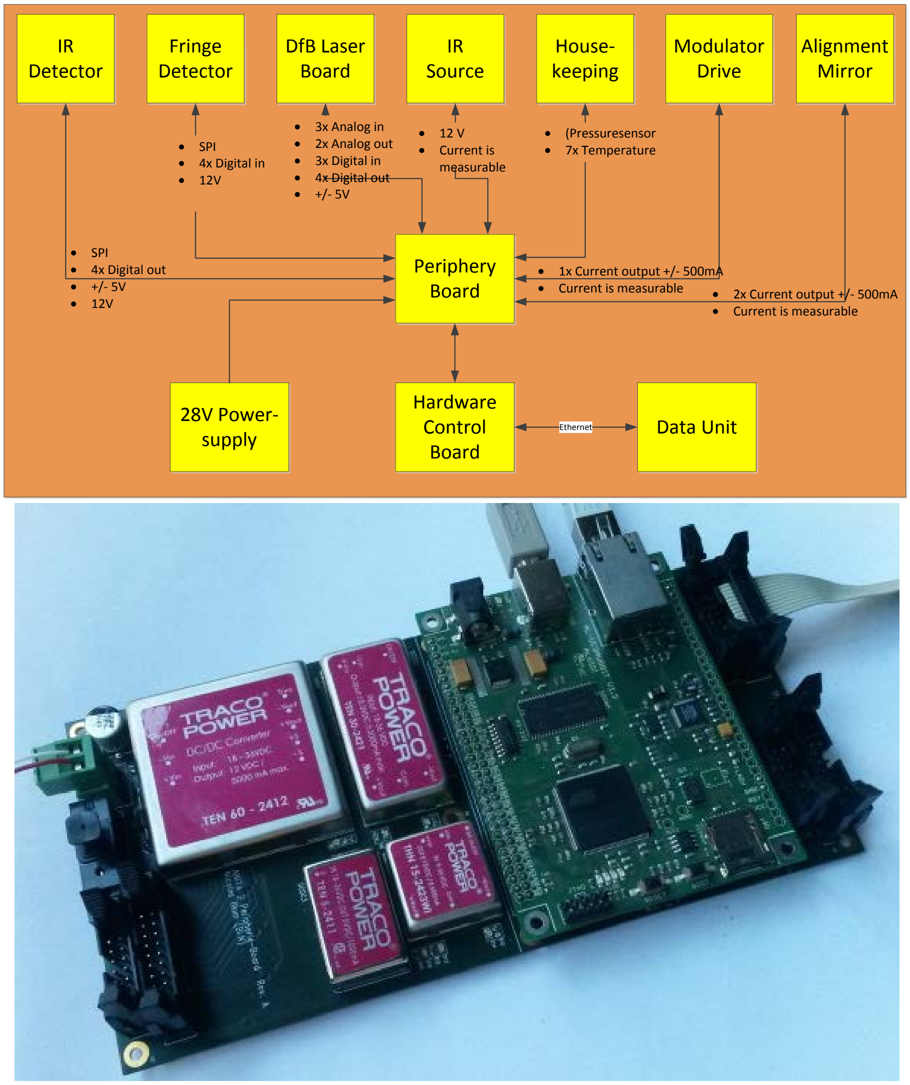

Figure 5: Electronic concept of ANITA2 (top) and integrated electronic board for the IBB (New Development).

C. Modulator Drive (New Development)

As described in previous papers, the FTIR modulator has been found as the most critical element in the new instrument design. The modulator is one of the main points of attention in this study, leading to the current breadboard presented here and finally to a totally new and more robust subsystem. The optical modulator is the core of an FTIR instrument. It represents a Michelson type of interferometer. The incoming optical signal is modulated by the movable mirror and the so-called interferogram is detected by a DLaTGS detector (Deuterated L-alanine-doped TriGlycine Sulfate). By the application of a mathematical transformation on the detected signal as a function of time – the Fourier Transform – the measured signal is transformed into a spectrum, which is used to execute the folowing gas analyses. Any micro-vibrations occurring in the system during the measurement cause tilts and shifts on the moved mirror, degrading the system performance. Based on the lessons learned in ANITA1 and on the pre-developments for the modulator of ANITA2, a new set-up of the modulator drive was developed, highly reducing the possible problem of micro-vibrations and mirror shifts and tilts. Figure 6 shows the newly developed ANITA2 modulator together with the previous version.

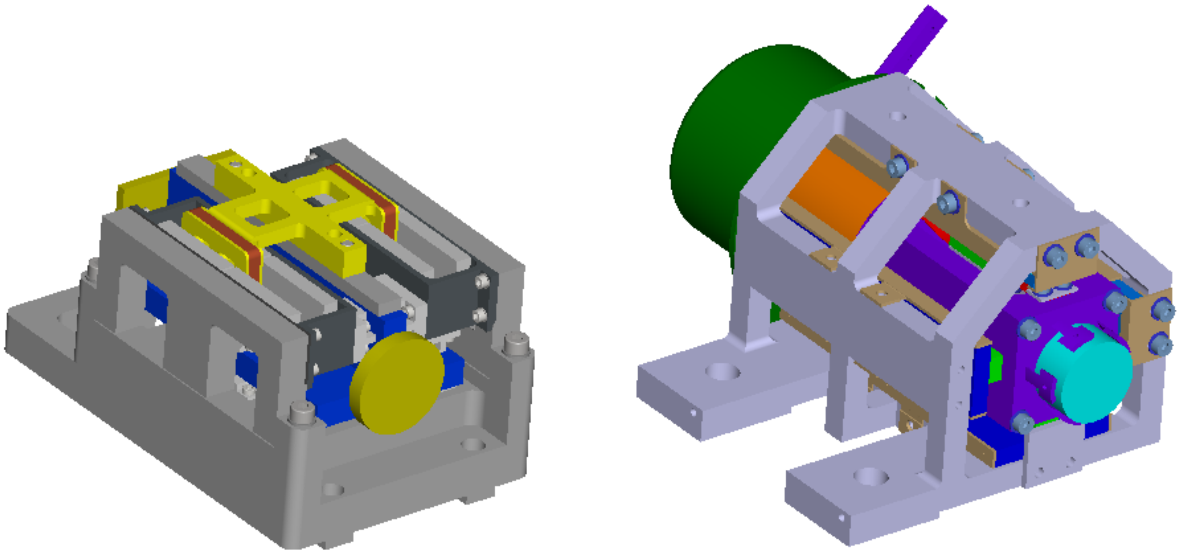

Figure 6: Design sketch of the new modulator (ver. 3) (left) compared to version 2 (presented in the previous paper).

The modulator is attached to the base plate by three bolts. This attachment allows an alignment of the modulator in all three translational and in all three rotational degrees of freedom.

The total weight of the new modulator is about 1.1 kg and is therefore much lighter than the ANITA1 system with about 4 kg and about 0.3 kg lighter than the version2 shown above on the right. The total weight can be reduced even further by special mass reduction measures on bulky materials.

D. Stabilized Laser Diode

For the achievement of the needed reduction in volume, mass and power consumption a temperature stabilized laser diode system had to be developed, replacing the bulky HeNe reference laser. The requirements on the frequency stability of the diode laser lead to the development and manufacturing of a customized analogue electronic board suitable for a DFB laser diode.

In order to reach the requirements of wavenumber stability better than $0.02\,cm^{-1}$ (goal requirement) for a maximum wavenumber of $\bar{\nu} = 4000\,cm^{-1}$ and achieve a wavenumber accuracy of better than $0.05\,cm^{-1}$ with an SNR greater than 3000 at $\bar{\nu} = 2200\,cm^{-1}$ for a measurement time of $t_m = 60\,sec$, the designed modules have to operate ultra-stable in scales of mK and mA.

The simulation of the current controller shows outstanding results with the response characteristics rise-time $t_r = 4.7\,\mu sec$, maximal over-shoot of only $1.1\,\%$, and a steady-state error less than $500\,nA$. This is while the simulation of the temperature controller results in a temperature stability of $1.351\,mK$ which is fully satisfying the goal requirement of $71\,mK$, with an over-shoot of only 0.12%. Actual long-term tests have been carried out on the final laser driver board to verify the board's functionality, for this purpose a wavelength-meter[13] is implied to analyze the wavelength stability while an optical powermeter[14] acquires the beam's intensity. The most important simulation and long-term test results can be found in Table 2.

[13] HP 86120B wavelength-meter, with resolution of $1\,pm$ and accuracy of $\pm 5\,pm$

[14] Ophir Pulsar-2 with a PD300-IR photo diode

Characteristic	Symbol	Value	Unit
Goal-required wavelength stability	$\Delta\lambda_{goal}$	4.26	pm
Measured wavelength stability	$\Delta\lambda_{meas}$	1.2	pm
Measured relative intensity stability	$\%\Delta I_{meas}$	0.644	%
Goal-required temperature stability	ΔT_{goal}	71	mK
Simulated temperature stability	ΔT_{sim}	1.351	mK
Measured temperature stability	ΔT_{meas}	4.398	mK
Goal-required current stability	ΔI_{goal}	1.42	mA
Simulated current stability	ΔI_{sim}	0.5	μA
Measured current stability	ΔI_{meas}	18	μA

Table 2: Summarization of requirements, simulation and the measured values by the long-term measurement.

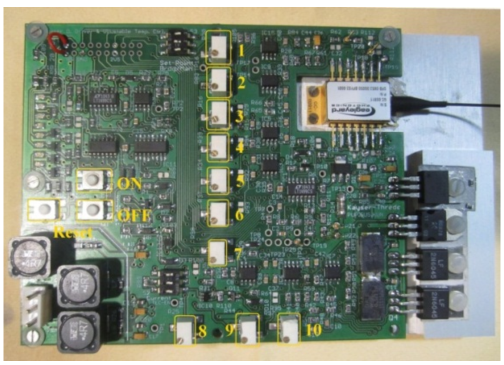

Figure 7: DFB Laser Board.

Figure 7 depicts the final integrated DFB laser board. The total mass and volume of the board are both around 10% of the mass and volume of the HeNe laser.

E. New IR Detector Board

The IR detector board uses a DLaTGS sensor to convert the optical signal into an electronic one. The resulting electrical signal will be amplified and digitized. In order to meet the new requirements a noise optimized circuitry was designed, and all data will be directly digitized on the board. All circuits and its components were simulated to ensure the performance before layout, design, and build-up. In addition a Thermo Electrical Cooler (TEC) was designed and implemented to control the Peltier element of the DLaTGS sensor and thereby the temperature of the sensor element. Due to that the sensor is always in the optimum temperature range with optimum performance. Figure 8 shows the final implemented detector board together with final schematics for explanation.

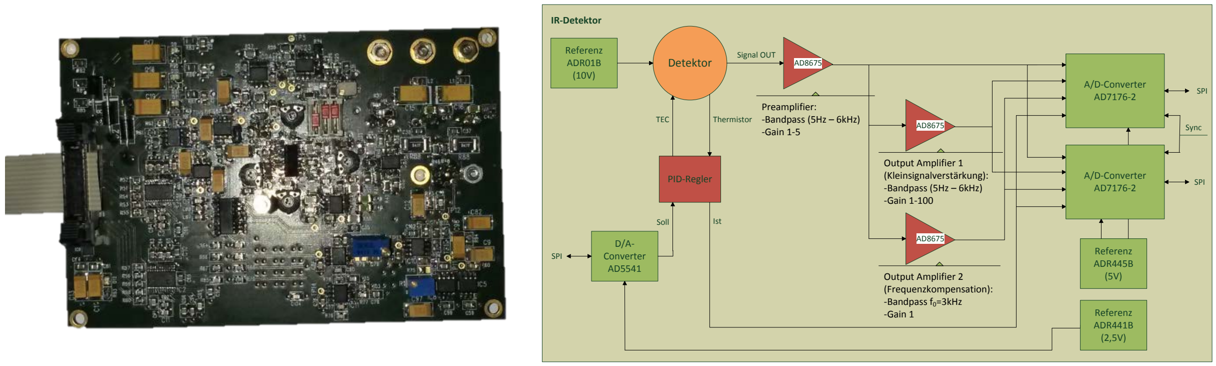

Figure 8: Final design of the IR Detector Board (right) and implementation with IR detector on the backside (left).

After integration the board was integrated in an optical test bench to validate its performance and to compare it with the old detector board of ANITA1. The results of these measurements are depicted in Figure 9 and Figure 10.

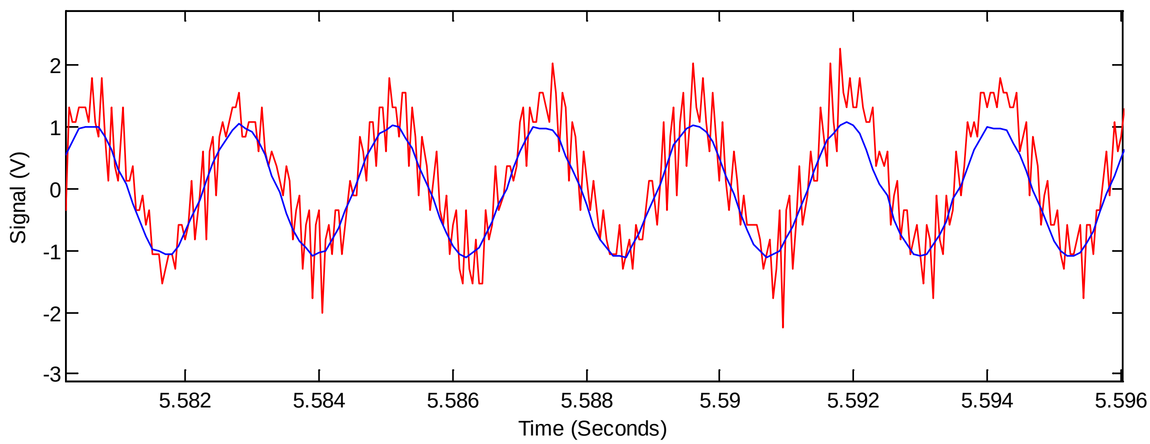

Figure 9: An extract of sample taken with the new detector board signal (blue) and the old detector board (red) with a chopper frequency of 442 Hz and an IR source voltage of 4V. Both signals are normalized to an amplitude of one. The new detector board signal contains much less noise than the old one.

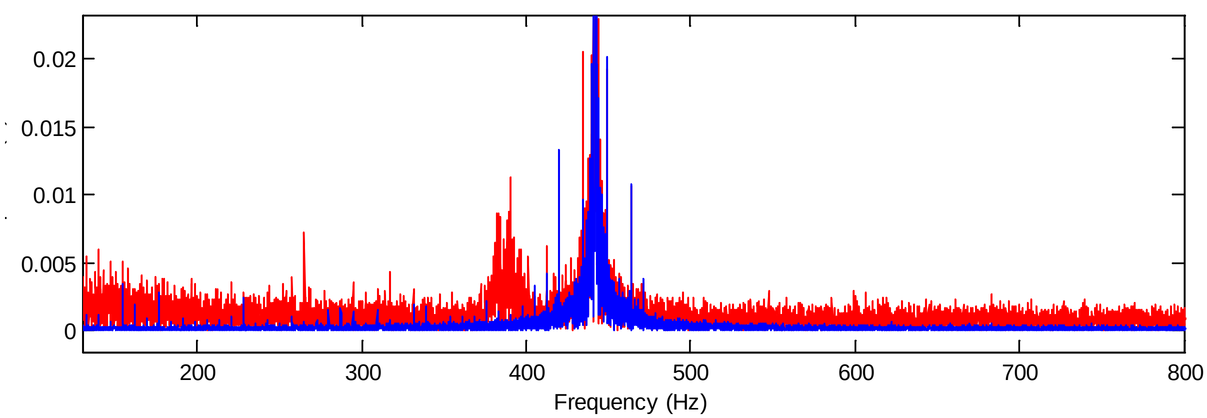

Figure 10: Spectrum of the measurement range (130 Hz – 800 Hz) with the signal peak at 442 Hz and normalized to an amplitude of 1. The spectrum of the new detector board (blue) contains significant less noise compared to the spectrum of the old detector board (red).

Detector Board	SNR Value
New IR Detector Board	635
Old IR Detector Board	55

Table 3: SNR values of the new and old IR Detector Board.

The table above shows that the noise performance and therefore the SNR of the new IR detector board is by a factor of 10 better than the old ANITA1 flight detector.

V. Experience with Gas Analyses in ANITA1

FTIR instruments have for a long time been well developed and established as efficient and reliable reference instruments in infrared spectroscopy. Owing to the good design and the built-in laser reference and optical compensations, high-quality infrared spectra can be produced. In multi-gas measurement, these spectra can resolve many of the unique spectral features for each gas. However, there are still two main types of challenges when we want to use the spectra to estimate gas concentrations. Firstly, the spectral features for the different gases are generally highly overlapping and tend to be overshadowed by each other and especially by the high-absorbing omnipresent background gases water vapour and carbon dioxide. Secondly, even high-quality FTIR spectra still exhibit measurement noise, baseline drift, optical saturation problems, and non-linear response.

In order to cope with these challenges, the novel techniques for gas analyses in ANITA were developed in several steps as part of and in parallel to projects for ESA. ANITA’s analysis software applies simulations of the measurement process followed by multivariate statistical analyses to produce calibration models that are pre-tuned to handle all the major problems of multi-gas measurement. This method of spectral analysis handles all the complexity of multi-gas measurement in the calibration process. Thereby, the runtime analysis of each measured IR spectrum can be made extremely fast and well suited for automation.

Through several development and implementation phases, two breadboard systems and finally the ANITA1 system were proven to work properly through testing on sets of accurately prepared multi-gas mixtures with known contents. In 2000 this was independently confirmed, when ANITA1’s precursor system came out on top in NASA's competitive blind testing of systems for multi-gas air analysis[1].

ANITA1 operated successfully on the ISS for 11 months in 2007 – 2008, performing fully automatic air monitoring of 33 gas components with high time resolution (cycle time 6 minutes). Despite several new challenges on board, ANITA1 could produce high-quality gas estimates, revealing new information on the ISS air contents and their dynamics. The main new challenges on the ISS were[1]

- One unexpected gas
- Spectral disturbances giving spectral artefacts and much higher spectral noise levels
- Small changes in spectral line shape (basic spectral response function)

The following two plots for Ethanol and Carbon Monoxide are illustrating results from previous cabin air analysis (2007).

These data are representing a comparison between results from on NASA onboard GS, analyzing so-called grab samples (cabin air from dedicated locations throughout the ISS) and the ANITA system of that time.

The black dots are indicating the GC data and the white circles are marking ANITA1 data gaps.

<u>Ethanol</u>

The overall comparison graph for ethanol is shown in Figure 11. Like for methanol, the general picture is that the two systems show good agreement, but the agreement is clearly poorer for the last grab sample. Also, relative to ANITA1, the last grab sample gives the clearly most negative deviation.

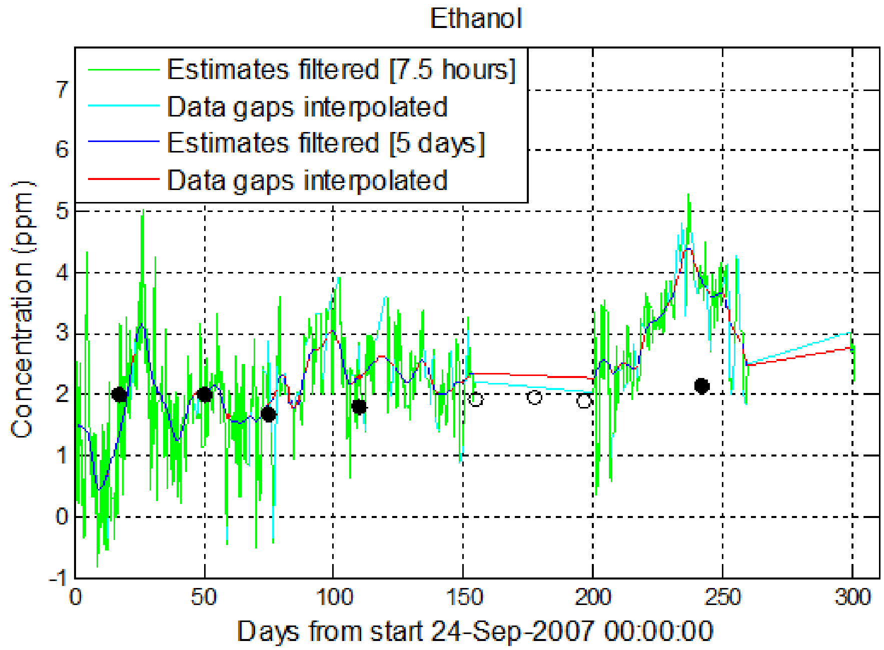

Figure 11: Ethanol: ANITA1 estimates with NASA's GC estimates indicated as black dots (open circles where ANITA has data gaps). Before the specified Gaussian filtering, there has been standard spectral sifting followed by filtering with a 5-point median filter for both traces.

<u>Carbon Monoxide</u>

In the comparison graph for carbon monoxide in Figure 12, all the grab sample data are marked as below the reported detection limit, and only one value is reported as "trace". For all the five comparable data points, the grab samples give no detection, and each data point in the graph is indicated as zero concentration with a bar up to the detection limit (0.5 ppm for the first sample and 0.25 ppm for the other four samples). From the graph, we can see that ANITA1 consistently measured higher values between 0.7 and 2.2 ppm, i.e. higher than the reported detection limit for GSC.

For further comparison, the CSA-CP also produces CO data. This system has a read-out resolution for CO of 1 ppm. It generally shows zero for CO with bounce to 1 ppm at times.

Carbon monoxide is a gas particularly well suited for measurement by ANITA1. The gas has a very distinctive spectral line pattern in a spectral area with moderate inter-gas interference, and also with very modest influence from ANITA1's spectral ghosts on the ISS.

ANITA1's curve for carbon monoxide relates well to known events on the ISS, most notably the hatch openings to visiting spacecraft. And the unexpected – and so far unexplained – concentration dip before the first Shuttle visit fits well with a parallel dip for methane. This combined dip for these two crew-related gases looks clearly significant, especially since there were no observed corresponding effects on other gases or on ANITA1's spectra. Thus, there are clear indications that ANITA1's carbon monoxide curve gives significant information, at least qualitatively.

With ANITA1 for all practical purposes out of physical reach on the ISS, all actions for compensation or adaptation had to be performed on ground or from ground. Owing to the flexibility of the simulation-based method of calibration, it was possible to produce updated calibrations to handle the problems.

Unexpected gases in the air, i.e. gases nor prepared for in the calibration, is a general and actually expected challenge. Whenever an improved or different gas monitoring system is introduced, or something new happens on the ISS, new gases may be detected. The challenges related to an unexpected gas are first to reveal a problem, then to diagnose the situation, then to identify the new gas, and finally to update the calibration. ANITA1 was well prepared for this and gave immediate warnings from ANITA1's automatic outlier warning system, which also automatically could highlight the spectral signature of a suspected "outlier gas". Therefore the new gas could quickly and easily be identified. Applying the standard calibration procedure, an updated calibration including the new gas was produced without access to the ANITA1 system. Initially this updated calibration was applied on ground, analysing current as well as historical spectra. Later the new calibration was uplinked to the ISS and installed through remote access to ANITA1 for regular, online use.

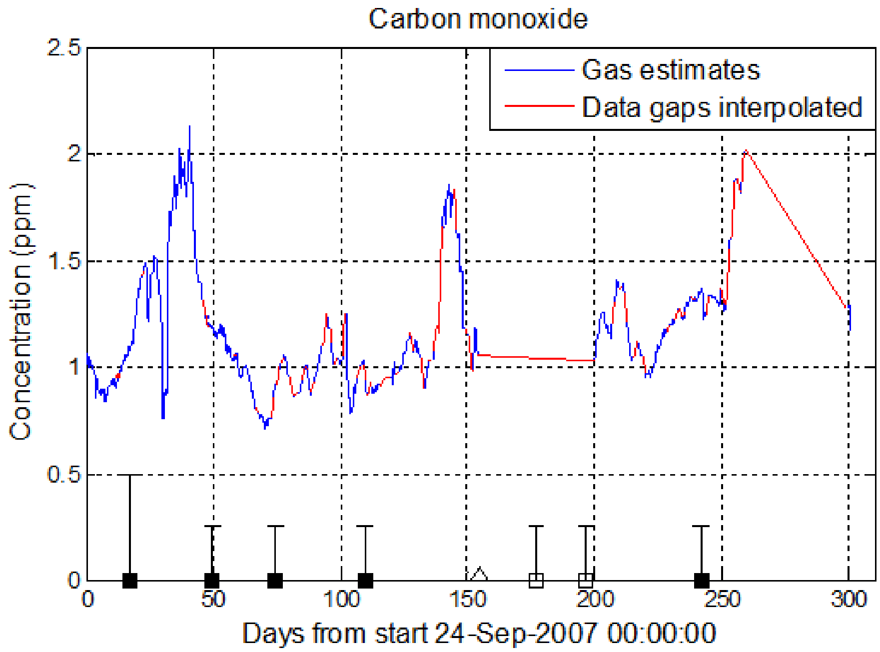

Figure 12: Carbon monoxide: ANITA1 estimates with NASA's GC estimates indicated as black data points (open where ANITA1 has data gaps). After standard spectral sifting, ANITA1's estimates have been filtered with a 5-point median filter and a Gaussian filter with FWHM 7.5 hours.

The technical problems related to spectral artefacts and excessive measurement noise in ANITA1 are believed to be caused by mechanical vibrations of unknown origin. The induced disturbances on the gas measurement were minimised through special adaptations of the updated calibration. Avoiding these problems is a key target of the ANITA2 hardware development.

ANITA1's spectral line shape surprisingly changed somewhat on a few occasions. This induced noticeable changes in ANITA1's concentration estimates for a few gases. These changes – presumably errors – were quite moderate; they just reduced ANITA1's advantage over alternative measurement techniques in terms of accuracy, reproducibility, and stability. However, a reduction in ANITA1's measurement quality could not be accepted without trying countermeasures. The line shape changes were successfully handled through adaptation of two parallel calibrations with different line shapes combined with automatic detection of the current line shape. For ANITA2, potential line shape problems will be reduced in two ways. Firstly, an even more stable instrument design will improve the line shape stability. Secondly, new ways for the analysis software to handle any remaining significant line shape variations are under development.

VI. ANITA2 Phase A Development of Gas Analyses

A. Background

Further phase A development of the gas analyses for the ANITA2 system is ongoing in the current project phase. The main target is to establish how any remaining variations in line shape can be handled in the best way.

In ANITA's calibration process, the multivariate statistical analyses can be tuned to sort out in an optimal way virtually all available information on gas concentrations. The quality of the results relies entirely on the quality of the input, i.e. the accuracy of the simulations of the measurement process. The calibration software for ANITA1 already simulated and handled in a good way the effects of several basic or instrument-induced phenomena like inter-gas spectral interference, non-linear spectral response, optical saturation effects, measurement noise, and instrument baseline drift. Since no problematic line shape variations were expected at the time, no countermeasures were prepared before the operation on the ISS. However, when changes in line shape were discovered and found to cause problems for ANITA1's gas estimations, an ad hoc solution was developed. This solution exploited the fact that the line shape was found to vary mainly between two modes, each with a specific line shape. This allowed a successful solution applying two parallel calibrations as an add-on feature.

Such a solution with parallel calibrations is guaranteed to work like standard calibrations, if the actually occurring line shapes can be implemented correctly in the calibration, and the current line shape for each measured spectrum can be identified correctly. The latter condition will cause a serious estimation problem owing to measurement noise, if each spectrum may exhibit a line shape that is unrelated to its preceding and following spectrum. If many – or at least several – spectra can be applied for each line shape estimation, this estimation can be quite reliable. This was the case for ANITA1 on the ISS, since the instrument only occasionally performed “mode hopping”. However, two or more parallel calibrations not only add to the complexity and extent of the calibration work, but it also gives a higher complexity for the runtime operation, especially regarding the line shape estimation. – For a normal calibration, the concentration estimate for each gas compound only involves a single vector multiplication of its calibration model and the measured spectrum, followed by a simple non-linear correction for a few gases.

The preferred ANITA approach to handle a phenomenon in the measurement scenario or in the instrument itself is to include it in the simulations. For line shape variations, this can be performed either through including different observed line shapes or through simulating small, theoretical variations around an observed line shape. The key to a good implementation is that the included line shape variations cover the future instrument behaviour.

Applying observed line shapes in a calibration requires that they are representative for the instrument under the relevant conditions. For a pre-launch calibration to be valid on the ISS, the relevant conditions must include any changes induced by transport, including the launch. A safer approach is to include only line shapes observed after start-up on the ISS. The downside will then of course be that it takes time to cover the relevant variations – for ANITA1 the first significant line shape change occurred after 46 days of operation. Therefore calibration updating must be foreseen. The most labour-intensive part of a calibration updating will be the surveillance of the spectra and the definition of the optimal input. As soon as the right input has been defined, implementing the calibration updating is a rather quick and easy procedure using ANITA's calibration tools.

If the calibration is based on simulated theoretical variations around an observed line shape, there is a larger risk that the simulated line shape variations do not cover the actual types or sizes of future variations in a proper way. The resulting built-in robustness towards line shape variations will depend on how well the actual line shape variations are covered. Therefore this solution, too, may be further optimised through a new, adapted calibration after some time of operation in the correct environment.

Built-in robustness towards line shape variations must, like any other built-in calibration robustness, come at a potential cost in terms of reduced measurement quality whenever the robustness is not required. On the other hand, when the robustness really is required, the improvement in measurement quality may be important. The potential cost increases when the prepared variation span increases. This potential cost can maximally constitute the loss in measurement quality for the combined models compared to models with perfect line shape matching. At some level, this cost will become too large to justify the use of a single calibration, so that parallel calibrations should be preferred after all, in order to secure the measurement quality.

B. Test calibration combining two observed line shapes

The key issue for a calibration combining two observed line shapes is of course how to implement it. A second important issue is how to perform proper testing of the results. From ANITA1 on the ISS we have numerous spectra with two main line shapes. This is a good setting for a combined calibration, but not for testing it. The potential testing has one basic and one practical limitation. The basic limitation is that we have no accurate and reliable external source of a defined "truth", i.e. which gas concentrations ANITA1 ideally should have measured. The practical limitation is induced by the on-board spectral artefacts and elevated spectral noise levels.

A better setting for testing is the pre-flight testing of ANITA1. Calibration and system testing, including measurements on 30 accurately controlled real gas mixtures, were performed at SINTEF in Norway. After the system had been sent to Kayser-Threde GmbH in Germany, we discovered that the spectral line shape had changed slightly, but significantly. Before system handover to NASA, ANITA1 was again sent to SINTEF for a retesting, including measurements on 15 of the original 30 gas mixtures. At that time we had established procedures for spectral transformations to transfer spectra from one line shape to another. The retesting showed that the spectral transformations enabled us to adapt to a new line shape, giving gas estimates better than ESA's specifications, but with a somewhat smaller margin than the original system testing. The line shape adaptation improves the measurement quality, but it cannot fully restore the quality achievable with a perfectly stable line shape. – According to this experience, we prepared a procedure to observe ANITA1's line shape on the ISS and to adapt the calibration. This adapted calibration worked excellently until the first line shape change after 46 days, when the procedure was repeated to make the second of the parallel calibrations mentioned above.

Three calibrations for ANITA1 have been compared in the current work:

- The standard pre-flight calibration matching the line shape of the system testing
- A calibration adapted to the line shape of the retesting
- A calibration combining both line shapes

To produce the retest calibration, we transformed all reference spectra and constructed the adapted calibration on them. (Each reference spectrum has been measured on a precisely known concentration of the target gas in nitrogen.) For the combined calibration we included the original as well as the transformed reference spectra in the simulations, preparing the combined calibration for both line shapes.

In order to test and compare the calibrations they were all run on four sets of spectra of real gases: The system test set of gas mixtures, the retest set, the set of original reference spectra, and the set of transformed reference spectra. For each set of spectra, the calibration models with the matching line shape were best, the combined models were only slightly poorer, and the models with mismatched line shape were poorest. This ranking according to measurement quality was quite obvious even before the testing – except that there in principle might be a risk that the combined models could be the poorest, owing to a bad idea or a poor construction. The result that the combined models proved to be only slightly poorer than the optimal ones was as intended and hoped for.

For a seemingly significant number of gases (i.e. beyond the general effects of noise in the wider sense), the combined models are actually better than the supposedly optimal models for the relevant line shape. This probably reflects that the spectra of each test set of real gas mixtures has small variations in line shape, so that the robustness of the combined models to some degree is exploited even within a single test set with presumably constant line shape.

The tested calibration combining two line shapes demonstrates that robustness to changes in the line shape of an FTIR instrument can be effectively implemented in a single calibration. For the moderate difference between the line shapes as observed for ANITA1, the loss in gas measurement quality caused by applying the combined calibration instead of the optimal calibration for each line shape is quite small. For line shape changes of this magnitude, combined models represent a very relevant solution. The combined models make the runtime software simpler than when alternative models are applied for different line shapes, and they also offer improved robustness to other small line shape changes resembling but differing from the varieties used in the calibration.

C. Further phase A development

In the current project phase a second type of test calibration will be developed and a few varieties implemented and tested. This calibration will be based on simulated theoretical variations around an observed line shape as explained above. If this approach gives results comparable to the calibration combining two line shapes, such a variability calibration may be the preferred solution in the future. It can be implemented right after the first use of a new instrument, but still be open for adjustment later. If a batch of FTIR instruments can be produced and lined up in a consistent way, it might be possible that a single variability calibration can be applicable to the whole batch.

VII. Further Development of Gas Analyses for ANITA2

The planned ANITA2 main programme will aim for three to five years of operation on the ISS, possibly extended until end of life for ANITA2 or the ISS. The gas analysis software will include several points of refinement of the gas measurements, further increased autonomy, and a higher level of analyses on the final measurement results.

ANITA2 will have a basic calibration to cover the foreseen general gas scenario, just like ANITA1. This is a robust calibration intended to cover all expected occurrences and variations of detectable gases in order to give undisturbed and fully valid gas estimates. However, as always for built-in robustness, the more gases and variations that must be handled in the calibration, the higher cost this robustness towards gas occurrences will have in terms of lower measurement quality for the gases that actually occur. Therefore the gas analyses for ANITA2 are planned to include several sets of calibration models for different gas scenarios and automatically choose the optimal calibration according to the total picture.

The planned types of calibrations to be included can be grouped as follows:

- Basic calibration covering all expected gas variations

- Local calibrations for local gas scenarios (easier scenarios allowing better sensitivity)
- Extended calibrations to cover additional gases
  - Special add-on calibrations for specific, maximally sensitive, and fully quantitative outlier gas detection
  - Special add-on calibrations for specific incident-based sets of additional gases
    (e.g. fires or specific leaks or malfunctions)

All calibrations can be updated from ground after installation on the ISS, and new varieties can be added. Since no comparable air monitoring system will be active on the ISS before ANITA2 starts operation, ANITA2's early measurements will be especially important for considering updating. The outlier detection system may signal the need for the basic calibration to be extended to include any new gas, like for ANITA1. Also, the observed gas scenario may indicate that a new local calibration should be optimised for the currently normal operation.

Each add-on calibration model or set of add-on models works technically like any other gas model inside a gas scenario. They give the optimal outlier detection for the relevant gas or set of gases without affecting the measurement quality of the standard (or local) calibration. However, totally unexpected gases may still emerge, and other measurement problems may occur. Therefore, ANITA2 will have an extended version of ANITA1's general outlier detection system based on analyses of the measured IR spectra. A key element is analyses on the residual spectrum, i.e. all parts of the measurement spectrum that cannot directly be explained by the absorption spectra of the gases that have been detected. Such analyses can reveal suspicious spectral features, possibly indicating an outlier gas, or spectral artefacts indicating possible instrument malfunction. Such analyses can be automated to give decision support, or ultimately to fully diagnose the situation. More specifically it is possible to indicate which gas estimates that may be disturbed by any given outlier situation.

Since ANITA1 was a system at test, measurement results were not made directly available to the ISS crew. ANITA1's user interface was only used on ground for presentation of gas estimates, possible outlier warnings, and results from automatic spectral processing to support outlier evaluation. For ANITA2 it is foreseen that the crew will at least have access to gas results and special warning signals. Historic data and trends can be presented. ANITA's high time resolution allows studies of the dynamics for gases with fast variations and can also be exploited through time domain filtering (including simple averaging) to further improve the noise level and sensitivity for gases with slower variations.

VIII. Envisaged ANITA3 Development

The envisaged ANITA3 system will aim at use e.g. in exploration missions and in possible bases on the Moon and Mars. Based on extensive experience from ANITA1 and ANITA2, the ANITA3 programme will introduce improvements mainly in the following areas:

- Shrinking of the system in terms of mass and volume, approaching shoe box size
- Reduced power consumption
- Improved autonomy through measurement robustness and automatic flexibility
  - Numerous add-on calibrations for specific, maximally sensitive, and fully quantitative detection of new gases
  - Several add-on calibrations for specific incident-based sets of additional gases
    (e.g. fires or specific leaks or malfunctions)
  - Extensive automatic spectral analyses for outlier detection, diagnosis, and warning
- A still higher level of analyses on and presentation of the final measurement results.

IX. Conclusion

The ANITA1 mission was a big success delivering continuous, outstanding data sets on manned space cabin air conditions on the ISS. The next generation of FTIR-based air monitoring is in the described breadboarding and design phase. In the ANITA2 design, all 'lessons learned' from the ANITA1 mission are considered, leading to more than 50% improvements in system mass and volume and an estimated performance of at least one order of magnitude in improvement compared to ANITA1. The new system is designated for autonomous operation on teh ISS with a lifetime of 3 years and an optional extension to over 5 years.

The technology is also a good candidate for future manned missions/stations to/on Moon and Mars. For this purpose the third generation system ANITA3 will have a further improved design, allowing much smaller volume and mass for the overall system.

Appendix 1

Compound		CUCL (ppm)	Estimated detection limit (ppm)
No.	Name		
1	methanol	70	0.10
2	ethanol	30	0.3
3	2-propanol (isopropanol)	30	0.5
4	1-butanol	50	1.0
5	formaldehyde	5	0.10
6	acetaldehyde	30	0.4
7	propionaldehyde	50	0.4
8	butyraldehyde	40	0.3
9	toluene	6	0.9
10	meta-xylene	15	0.4
11	ortho-xylene	6	0.4
12	para-xylene	20	0.2
13	ethyl benzene	20	0.9
14	ethyl acetate	5	0.3
15	n-butyl acetate	4	0.2
16	dichloro methane	12	0.3
17	Freon 11	2	0.013
18	Freon 12	1	0.04
19	Halon 1301	1.25	0.05
20	Freon 113	3	0.05
21	perfluoro propane	100	0.03
22	hexane (n-)	12	0.3
23	acetone	10	0.4
24	2-butanone	30	0.3
25	hexamethyl cyclo-trisiloxane	2	0.003
26	octamethyl cyclo-tetrasiloxane	1.2	0.003
27	decamethyl cyclo-pentasiloxane	1	0.012
28	ammonia	4	0.06
29	carbon monoxide	10	0.05
30	methane	500	-
31	carbon dioxide	10000	-
32	water	25028	-

Table 4: Gas scenario and test results from the physical testing of ANITA1 on real gas mixtures. For each compound the columns show the gas number, gas name, CUCL (Calibration Upper Concentration Limit), and the estimated detection limit (ISO 95% confidence).

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