

ANITA Air Monitoring on the International Space Station

Part 2: Air Analyses

A. Honne, H. Schumann-Olsen, K. Kaspersen and S. Clausen
SINTEF, Norway

H. Mosebach, D. Kampf and T. Stuffer
Kayser-Threde GmbH, Germany

W. Supper and G. Tan
ESTEC, Noordwijk, The Netherlands

Copyright © 2008 SAE International

ABSTRACT

After the launch to the ISS (International Space Station) with The Space Shuttle flight STS 118 13A.1 on August 9th 2007 and the accommodation in the US lab Destiny, the air quality monitor ANITA (Analysing Interferometer for Ambient Air) has been successfully put into operation. ANITA is a technology demonstrator flight experiment being able to continuously monitor with high time resolution the air conditions within the crewed cabins of the ISS. The system has its origin in a long term ESA technology development programme. The ANITA mission itself is an ESA-NASA cooperative project. ESA is responsible for the provision of the HW, the data acquisition and data evaluation. NASA's responsibilities are launch, accommodation in the US Lab Destiny, operation and data download.

The ANITA air analyser is currently calibrated to detect and quantify online and with high time resolution 33 gases simultaneously with down to sub-ppm detection limits. In addition the system has automatic warning capabilities covering possible malfunctions, surprising gases, and gas concentrations above preset limits. - However, owing to the experimental character of this ANITA mission, no measurement results are on-line visible to the crew.

ANITA's standard, fully automatic mode of operation applies direct air sampling in front of the system. Whenever wanted, air samples for automatic analyses can be taken from any human-accessible position in the ISS or any connected spacecraft and fed to ANITA, applying gas bags and a hand pump.

ANITA is an on-orbit test experiment and a precursor for a permanent continuous trace gas monitoring system on the ISS - ANITA II. It further represents a precursor system for future air monitoring in crewed vehicles being

developed for the Human Space Exploration programme.

This paper is part 2 in a series of two papers. The first paper describes the HW and the ANITA mission itself. This paper is dedicated to the data analysis, including the handling of special challenges and some measurement results.

On the ISS, ANITA has measured several gases that, before now, have never properly been measured before, including one unexpected gas. And many gases have for the first time been measured with high time resolution. The observed gas dynamics clearly show effects from spacecraft visits to the ISS, crew activities, the number of crew present, and the functioning of the air revitalisation systems. ANITA gives detailed time-resolved information on very different gases such as carbon dioxide and monoxide, methane, ammonia, perfluoro propane, sulphur hexafluoride, siloxanes, and alcohols.

It was also demonstrated how ANITA was used to detect and quantify an unexpected gas in the ISS air, and how the system calibration could be updated from ground.

The work described has been performed under contract of the European Space Agency.

INTRODUCTION

Through a long term technology development programme starting in 1991 [1-9, 11, 13-20], the European Space Agency ESA has selected the FTIR (Fourier Transform Infrared) technology to continuously monitor the crewed spacecraft atmosphere quality. Based on different study and breadboard activities, supported by a very successful blind sample testing for NASA [10, 12], it was concluded that the requirements

for on-line multi-gas air analyses are best fulfilled by this optical detection method in combination with sophisticated analysis SW.

The system's measurement principle is detection of the infrared (IR) absorption features stemming from the different gas molecules' vibration/rotation modes. From the measured IR spectra the gas concentrations are derived via sophisticated analysis SW, which is briefly described below. 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.

INITIAL SYSTEM CALIBRATION

BASIS FOR THE CALIBRATION

The basis for and input to the system calibration includes:

1. Gas scenario
2. Measurement conditions
3. Ideal instrument response
4. Non-ideal instrument behaviour
5. Reference spectra

Items 1 and 2 for ANITA on the ISS are described in detail in [18].

The gas scenario is a list of all gas compounds that are expected or suspected to occur in significant concentration in the cabin air and a CUCL (Calibration Upper Concentration Limit) for each gas. A significant concentration means that the IR absorption of the gas may allow detection of that gas or inflict disturbances on the measurement of other gases.

The measurement conditions include the air temperature and pressure, in the space cabin as well as inside the gas cell of the instrument, and also the conditions for the routine background measurements. - In order to avoid the use of consumables on the ISS, ANITA uses local air pumped down to low pressure for background measurements instead of clean nitrogen. In addition, ANITA's spectrometer box is not allowed to be airtight for safety reasons. It therefore contains real air unintentionally sampled from the various surroundings whenever the safety valves have opened up for air influx. This is reflected in the rather heavy absorption in the background spectrum; mainly from water and carbon dioxide, as shown in Figure 1.

Items 3 and 4 are necessary input to simulate the instrument behaviour. Important aspects of the ideal instrument response include saturation effects as well as non-linear response caused by limited spectral resolution. In the simulations, the most important aspects of the non-ideal instrument behaviour are the stochastic noise (photon noise, detector noise, noise from the electronics) and the baseline drift.

The most important basis for the calibration is at least one reference spectrum for each gas compound in the gas scenario. The reference spectrum has been measured on the FM (ANITA Flight Model) itself at an optimised concentration, i.e. a compromise between local SNR (Signal to Noise Ratio) in the spectrum, saturation effects, possible non-linear effects, and the accuracy of mixing of the reference gas mixture. For gases where significantly non-linear response may occur, several spectra have been measured at different concentrations. This allows for simulation of the non-linear behaviour as well as correction of the gas estimates.

All the items 1 through 5 are important as basis for the simulations in step A in the next subsection.

THE CALIBRATION PROCESS

The main calibration process steps and methods can be roughly grouped as follows in the order they are applied in the calibration process:

- A. Simulations of measurement IR spectra
- B. Pre-processing of the simulated measurement IR spectra
- C. Statistical analyses applying PLS (Partial Least Squares)
- D. Corrections for non-linear characteristics

A basic tool is the PLS of step C. It is a family of multivariate statistical methods [21], which makes it possible to use examples (IR spectra for known gas mixtures) to find the best utilisation of information through avoiding disturbances and handling statistical noise optimally. The applied tool is denoted PLS1, which produces a separate calibration model for the concentration of each gas compound, taking into account the possible influence from all other effects that are represented in the examples.

The rather large set of examples (at least many hundred spectra) that is necessary for multi-gas calibration can for practical and economical reasons only be produced through simulations (step A). The simulations apply properly prepared reference spectra for the pure compounds, combine these to represent different gas mixtures, and impose all important instrument effects to produce realistic IR spectra. Thus the quality of the instrument calibration relies heavily on the adequacy of the simulations.

The simulations in the calibration process include concentration variations for all gas compounds between zero and their individual CUCL values. In the ANITA calibration, equal weight is put on all concentrations and combinations, giving a calibration that is fully robust for all possible air mixtures within the defined gas scenario. This calibration procedure gives a general set of calibration models that is always applicable, as long as the real air contents are within the simulation scenario. If any of the gases should exceed the limits of

the specified gas scenario, the measurement system will show a graceful degradation, i.e. a gradual (and generally very slow) loss of measurement quality without any point of breakdown.

Even though a PLS system can handle noise (measurement noise and other kinds of disturbances) in an excellent way, the modelling is hampered or possibly impaired by any unnecessary noise. Therefore, the pre-processing in step B enhances the PLS modelling by selecting spectral areas and by excluding data points with unwanted properties such as possibly too high absorbance (optical saturation) or excessive non-linearity.

Since PLS analyses inherently are linear, some of the handling of non-linearities must be implemented in an additional calibration step D as corrections after the application of the PLS.

FEATURES OF THE CALIBRATION

As a result of the described method of calibration the general features of the resulting calibration include:

- Control of optical spectral interference (the main problem)
- Baseline drift compensation (solves a major problem, since the “true” baseline cannot be observed or synthesised)
- Optimal noise handling utilising information from numerous spectral data points
- Control of possible optical saturation effects (too high spectral absorption)
- Simple, fast, and fully automatic runtime calculations (all complexity is handled in the calibration process)
- Easy adaptation to new measurement situations through recalibration, even after deployment in space (without astronaut involvement).

In addition to the general features, the ANITA calibration includes other mechanisms (see above and [17]) like special handling of non-linear spectral interference, automatic correction for non-linear gas response, outlier detection, and local calibration models for even better sensitivity.

The approach of applying simulations ensures close to optimal extraction of spectral information given the simulated effects. However, any disturbance *not* included in the simulations is implicitly assumed as non-existing, and no protection or compensation is achieved.

SYSTEM TESTING

The strategy for the initial system testing of ANITA before acceptance for flight has been:

- Extensive synthetic testing (simulated measurements)
- Moderate, but still convincing, system testing (measurements on real gas mixtures)

Details on the test procedures and test results are given in [18]. The conclusion from the testing was that ANITA fulfilled ESA's requirements for gas analysis with a considerable margin.

UNEXPECTED GAS ON THE ISS

OUTLIER GAS DETECTION

An *outlier gas* is a gas compound that ANITA is not calibrated for, because it was not expected to occur in significant concentration to be detected or to disturb the measurements. The outlier detection subsystem in ANITA has been described earlier (see [8] for basics, [16] for special improvements, and [19] for implementation and use in ANITA).

When the first measured spectra came in from the ISS, they were also run offline on ANITA's user interface on ground in the Mission Control Center at JSC (NASA's Johnson Space Center). The system gave outlier warnings based on several outlier criteria. In order to assess the root cause of the outlier situation, the Gas Plots dialog was selected as shown in Figure 1. In the bottom plot, the spectral areas with non-nominal behaviour are highlighted in red.

Although the unexpected noise levels (see next chapter) also contributed to this non-nominal spectral behaviour, it is quite typical that a local spectral outlier feature may lead to non-nominal behaviour also in other parts of the spectrum. This is caused by erroneous gas estimates induced by the primary outlier feature. This spectral feature inflicts disturbances upon the estimates of all gases with calibration models covering the spectral area in question. The disturbances may be positive or negative depending on each model. Any significantly negative gas estimate in itself gives rise to an outlier warning. Any significantly increased gas estimate will add to the synthetic spectrum and give too high subtraction from the residual spectrum. And this extra subtraction will happen in all spectral areas where the overestimated gas exhibits optical absorption.

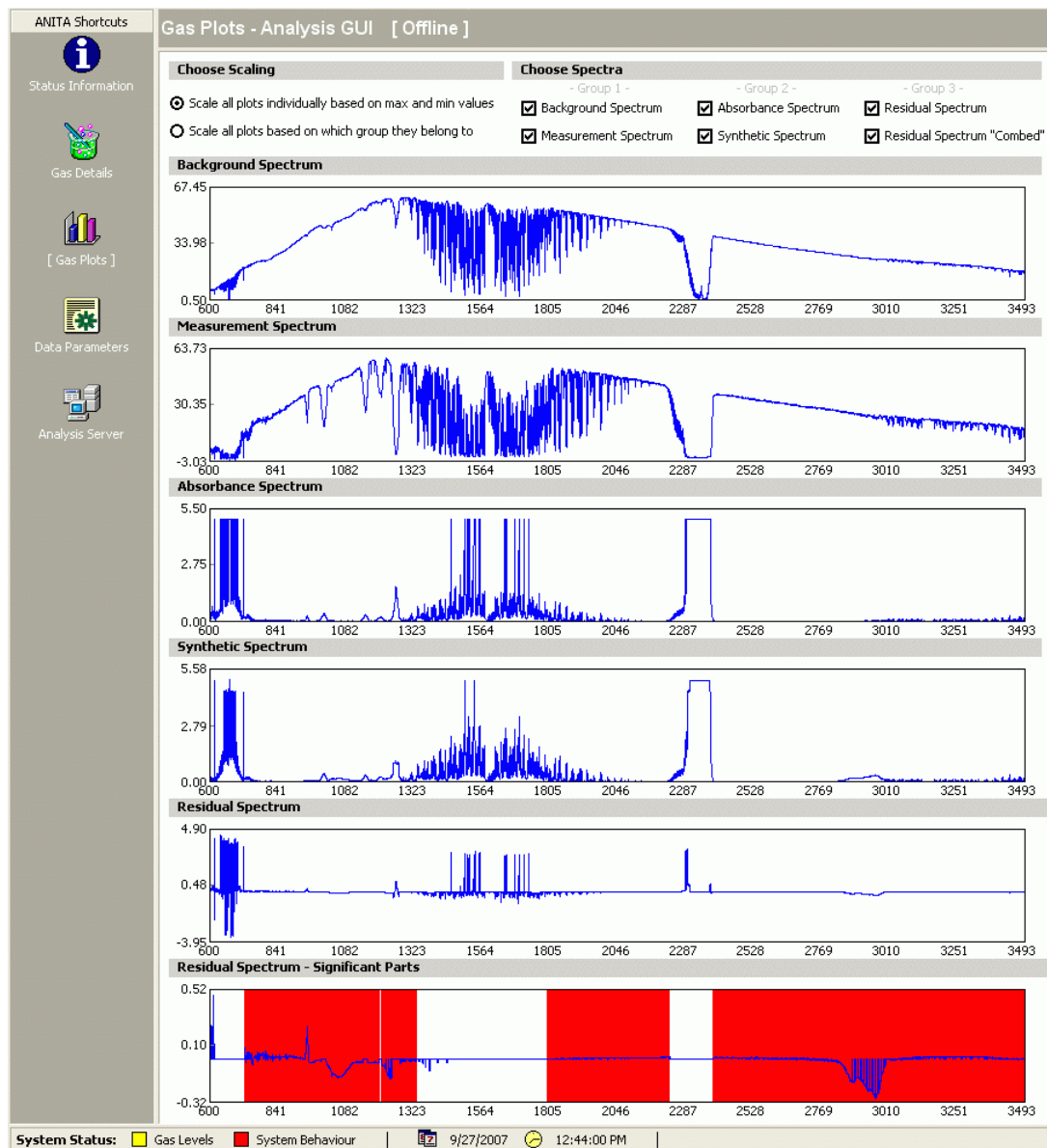


Figure 1. Screenshot from the ANITA Analysis Software user interface on ground. The selectable Gas Plots dialog is shown for the analysis of an early measurement on the ISS. The plots show from top to bottom the measured background spectrum, the foreground spectrum, the calculated absorbance spectrum, 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 of the plots has been 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). Please see the text for discussion on the analysis output.

In the bottom plot of Figure 1, the negative spectral features must be caused by excessive subtraction of the supposed absorption from gases that have been overestimated. The most promising clue for revealing any outlier gas is the only positive peak right below 950 cm^{-1} .

A simple search on the Internet for an absorption feature in this position gave sulphur hexafluoride, SF_6 , as a good candidate for an outlier gas. When we compared our library spectrum of SF_6 with the spectral feature in

the residual spectrum and in the measured absorption spectrum, it was obvious that we had detected SF_6 as an unexpected gas.

Since the absorption feature was very significant in the measured spectrum, it was possible to estimate the concentration of SF_6 to 0.7 ppm by the classical peak estimation method, relying on the believed true concentration*path product of the library spectrum. – When we later made our own controlled gas mixtures and measured reference spectra (see Figure 2) for a

final calibration, this estimate was adjusted to about 1.1 ppm (see below under results).

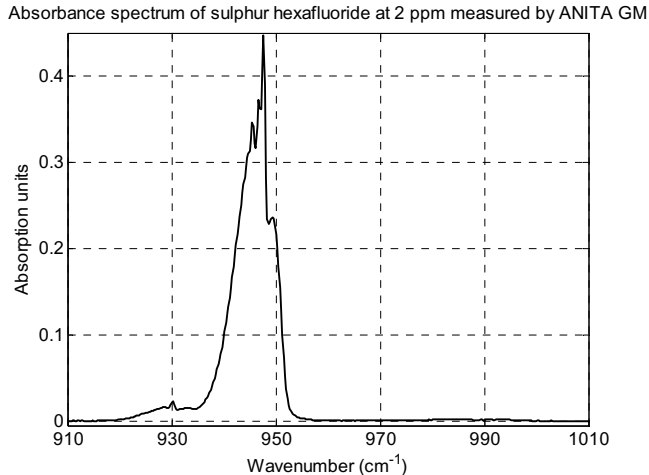


Figure 2. Spectrum of SF₆ at 20 ppm*m from ANITA GM, showing the non-negligible features within the spectral area applied by ANITA (in total 650 – 3500 cm⁻¹)

The detection of SF₆ was a total surprise. However, SF₆ is an entirely harmless gas that hardly interacts with anything other than IR radiation, making it a very potent greenhouse gas as well as a suitable test and tracer gas. And a question to NASA quickly revealed that SF₆ actually is applied on the ISS for calibration of a medical experiment (Periodic Fitness Evaluation with Oxygen Uptake Measurement, PFE-OUM)). And owing to its inertness, it tends to stay in the cabin air.

PRELIMINARY CALIBRATION

In general, library spectra cannot be applied as reference spectra for a proper calibration of ANITA's type, because the wavenumber scale as well as the line shape may not fit. It also happens that library spectra are composed of parts of different spectra with non-matching parameters. In addition, library spectra may have been manually "cleaned up" by zeroing noisy areas with the risk of removing significant features as well.

Before a set of proper reference spectra (more than one to handle non-linear response) could be measured, a preliminary solution was implemented. This solution was possible because SF₆ only has one rather narrow spectral band in the relevant spectral area. In the modelling tools, this band covering 920 to 954 cm⁻¹ was manually zeroed out to be handled like other spectral areas with unwanted properties. Thereby a preliminary calibration could be produced on the spot. This calibration removed most of the effects of SF₆ as an outlier gas, restoring the calibration for the original gas list. However, this calibration did not include any model for SF₆, which still had to be estimated manually with the classical method as described above.

In retrospect it is interesting to see that our library spectrum (of generally recognised quality) for SF₆ had been too much cleaned up. The rather weak band around 990 cm⁻¹ in Figure 2 had been zeroed out. At the concentrations we encounter on the ISS, this weak band is still quite significant to disturb the calibration. – If a calibration is good enough to utilise low-absorbing features, it can also be disturbed by such features, unless they are included in the calibration simulations.

FINAL CALIBRATION

In order to measure a proper set of reference spectra, we must apply a suitable FTIR instrument and a vacuum system for accurate gas mixing. Initially, ANITA's Ground Model (GM) had to be at JSC for troubleshooting purposes during the start-up and the early operational phase for ANITA on the ISS. The combination of necessary equipment was therefore not available in one place before the GM could be sent to SINTEF.

Although the GM is close to a twin of the ANITA system on the ISS, it does not produce identical spectra. The differences in line shape were handled through special spectral transformations based on the methods in [22].

With a set of proper reference spectra for SF₆, an extended calibration was produced, including SF₆ as gas number 33 in the gas list. When all measured spectra were re-run on the new set of calibration models, all gases in the extended gas list were properly estimated with the full time resolution available in the first place.

SPECTRAL DISTURBANCES ON THE ISS

SPECTRAL DISTURBANCES

The selection of the measurement technology as well as the calibration of ANITA is based on the exceptional quality of the FTIR spectra in terms of stability as well as SNR. However, when the system was put into operation on the ISS, severe disturbances in the measured spectra were observed. Analyses on the disturbances revealed that they had a high degree of structure, but still with a high variability, as shown in Figure 3. The structure suggests a high impact from spectral "ghosts", i.e. spectral features that erroneously reappear at different positions in the measured spectrum. In the shorter term, normally from hours to days, possibly weeks, the variable pattern typically has a rather fixed position in the spectra like in the plot. Over longer time the spectral features also tend to move along the wavenumber axis.

The source(s) of the disturbances and their propagation into the measured spectra are being analysed. However, this diagnosis work depends on non-standard information from ANITA on the ISS as well as the local environment that at the time of writing are very difficult to trace.