

Evaluation of ANITA Air Monitoring on the International Space Station

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ABSTRACT

ANITA (Analysing Interferometer for Ambient Air) is a flight experiment precursor for a permanent continuous air quality monitoring system on the ISS (International Space Station).

For the safety of the crew, ANITA can detect and quantify quasi-online and simultaneously 33 gas compounds in the air with ppm or sub-ppm detection limits. The autonomous measurement system is based on FTIR (Fourier Transform Infra-Red spectroscopy). The system represents a versatile air quality monitor, allowing for the first time the detection and monitoring of trace gas dynamics, with high time resolution, in a spacecraft atmosphere.

ANITA operated on the ISS from September 2007 to August 2008. This paper summarises the results of ANITA's air analyses and compares results to other measurements acquired on ISS during the operational period. The main basis of comparison is NASA's set of grab samples taken onboard the ISS and analysed on ground applying various GC-based (Gas Chromatography) and GC/MS (Mass Spectrometry)

systems. Comparison with other real-time instruments aboard ISS included the Volatile Organic Analyzer (VOA), the Compound Specific Analyzer – Combustion Products (CSA-CP), the Carbon Dioxide Monitor (CDM), and the Major Constituent Analyzer (MCA).

INTRODUCTION

ANITA represents the current status of the European Space Agency ESA's long term technology development programme for continuous monitoring of the atmosphere quality in crewed spacecraft [1-9, 11, 13-22]. At an early stage, the FTIR technology combined with sophisticated multivariate statistical data analyses was selected as the most promising solution. Based on various 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 combination of techniques.

The launch of ANITA to the ISS was performed in August 2007 by the Space Shuttle Endeavour flight STS-118. ANITA was set up in an EXPRESS rack in the US module Destiny aiming for six months of operation, and the system start-up took place in September. Thanks to

ANITA's successful operation on the ISS, giving new and very valuable information on the gas status and air dynamics in the spacecraft air, the operation was prolonged until August 2008. Then, further operation was no longer possible, because of a long-planned relocation of the payload rack infrastructure on the ISS.

The ANITA mission itself was an ESA-NASA cooperative project. ESA was responsible for the provision of the HW, the data acquisition and data evaluation. NASA's responsibilities were launch, accommodation in the US module Destiny, operation, and data download.

ANITA's standard, fully automatic mode of operation applies direct air sampling in front of the system. Whenever wanted during the mission, air samples for automatic analyses could be taken from any human-accessible position in the ISS or any connected spacecraft and fed to ANITA, using gas bags and a hand pump. However, owing to the experimental character of this ANITA mission, no on-line measurement results were visible to the ISS crew.

The current ANITA calibration prepared it to detect and quantify, quasi-online and simultaneously, 33 gas compounds in the air down to lower sub-ppm detection limits. In addition the system has automatic warning capabilities covering possible malfunctions, unexpected gases, and gas concentrations above preset limits. Immediately after the system start-up on the ISS, it was demonstrated how ANITA could be used to detect and quantify an unexpected gas in the ISS air, and how the system calibration could be updated from ground [22].

ANITA'S MISSION ON THE ISS

ANITA CALIBRATION FOR THE ISS

Before the ANITA mission, the system was calibrated for the expected worst case gas scenario on the ISS [18]. The gas scenario is defined through a list of all gas compounds, plus their individual upper limit of concentration variations, that are expected or suspected to occur at significant concentration in the cabin air. A significant concentration means that the IR absorption of the gas may be large enough to allow detection of that gas or large enough to inflict disturbances on the measurement of other gases through spectral interference (cross-sensitivity), unless it is prepared for through the calibration process.

The occurrence of an unexpected gas, i.e. a gas not in the gas list, may introduce interference on the measurement of other gases through spectral overlapping that has not been accounted for in the calibration process.

A central tool of the calibration modelling is PLS (Partial Least Squares). It is a family of multivariate statistical methods [23], which makes it possible to learn from examples how information can be extracted from data

sets in an optimal way. For ANITA, IR spectra for known gas mixtures constitute the examples, and PLS is applied to find the best utilisation of information through avoiding spectral interference 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. Although PLS is very effective optimising the extraction of information, it is very advantageous to perform data pre-processing in order to apply any pre-knowledge of where in the spectrum useful information can occur.

A sufficiently large example set of IR spectra (hundreds) for very accurately known real gas mixtures can hardly be produced. The examples must be constructed through simulations. Therefore we must be able to describe and simulate the instrument behaviour, applying proper reference IR spectra for all gases involved, the ideal instrument response, as well as all foreseeable varieties of non-ideal behaviour.

In summary, the calibration of ANITA was performed through four main steps [22]:

1. Simulations of measurement IR spectra
2. Pre-processing of the simulated measurement IR spectra
3. Statistical analyses applying PLS
4. Corrections for non-linear characteristics

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

- Control of optical spectral interference (cross-sensitivity between gases, 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)
- Semi-permanent calibration: No recalibration is necessary unless the gas scenario or the instrument changes beyond the specifications
- Easy adaptation to new measurement situations through recalibration, even after deployment in space (without astronaut involvement)
- All complexity is handled in the calibration process. The runtime calculations are simple and very fast.

The potential for a semi-permanent calibration relies on the inherent optical compensation for intensity changes (aging or contamination of IR source, optics, or detector) and the excellent FTIR wavenumber stability achieved through the built-in laser reference.

In addition to these general features, ANITA's calibration includes other mechanisms [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.

ANITA OPERATION ON THE ISS

After the system set-up on the ISS, the FTIR moving mirror could not be started [21]. Here, repeated power cycling led to a warming up and finally to the successful start of the system. After this, ANITA produced measurement data most of the time. However, problems mainly with the ISS laptop PC dedicated to ANITA led to periods of missing data, which are referred to as "data gaps" below.

From the very first measurement on the ISS, ANITA gave outlier warnings, indicating that something was out of specification. ANITA's outlier analysis features revealed that the problem was an unexpected gas that could be identified as sulphur hexafluoride (SF_6). This situation was resolved through recalibration from ground [22]. – The gas SF_6 is an infrequent contaminant with extremely low toxicity that is used in specific medical investigations. Therefore it had not been among the target gases of earlier analyses of the ISS air. Consequently its presence in the ISS air was unknown, and the gas was not included in ANITA's gas list.

In addition to the unexpected gas, a few technical surprises occurred on the ISS. The spectrometer's spectral line shape changed slightly through some of the system restarts, and the spectra contained unexpectedly high levels of noise in addition to variable spectral "ghosts" (spectral signals that falsely reappear in other positions in the measured spectrum) [21, 22]. At the time of writing, these technical problems are still under investigation, since the ANITA system has only recently been returned after the mission.

The variable line shape was handled through special calibration modelling that apply spectral transformations (developed based on [24]) in order to match dedicated calibration models to the different line shapes. The noise and ghost problems were minimised through calibration modelling optimised for higher robustness, spectral sifting (automatic rejection of spectra with very poor quality), and time domain filtering of the gas estimates (optimised weighted averaging) [22]. In total, the applied adaptations and countermeasures were highly successful, ensuring valuable data from ANITA.

POST-PROCESSING OF ANITA DATA

Depending on the observed, assumed, and/or accessible frequency contents of the time series, each gas has its special selection among the treatments spectral sifting, median filtering, and Gaussian filtering with a selected filter width (defined as FWHM – Full Width at Half Maximum) [22]. The applied data treatment for each gas

is specified in the text of each graph below. This treatment is quite different for the different gases, trying to preserve potentially valuable information on the fastest significant variations that can be extracted out of the noisy primary gas estimates.

"Sifting" of the spectra implies removal of all spectra falling below a pre-set quality limit for each of a number of parameters derived from each spectrum. This standard sifting removes the 34.6 % poorest spectra out of the initial 6398 spectra downlinked from the ISS.

In order to improve potential outliers in the gas estimates, most gases have been filtered with a sliding 5-point median filter, ignoring missing data points.

For time domain averaging filters, we have applied Gaussian filters of different widths, taking missing data points into account (i.e. preserving the correct time scale in the filtering). The FWHM (Full Width at Half Maximum) for each filter is given for each graph.

The significance of gas concentration curves after filtering is of course quite different from the significance of each individual primary gas estimate. With increasing time averaging, the stochastic noise is increasingly suppressed, and offset and stability of the system become increasingly important as limiting factors.

For some gases, two different levels of time averaging (Gaussian filters with different widths) are shown in the same graph for maximum usable information – including information on the noise level. This twin treatment has typically been applied for gases where fast variations should be expected in reality, but where the overall spectral noise leads to poor significance for the estimates on these fast variations. – E.g. for ethanol (see Figure 5 and Figure 9), it is reasonable to expect relatively fast variations owing to human activities. However, the occasional negative values in Figure 9 definitely indicate a problem with the significance for the least filtered curve, especially early in the flight, when the ghost problem was most severe for this gas. Heavier filtering evidently leads to better significance while hiding all information on fast variations in gas concentration.

The following widths (FWHM) were chosen for the applied Gaussian filters for different gases:

- 40 min (alone: No sifting or median filtering): Water and PFP (perfluoro propane, Freon 218)
- 2.9 hours (alone): CO_2 . Preserves the shape of daily concentration "valleys"
- 7.5 hours, after sifting and median filtering: 8 gases
- 5 days, after sifting and median filtering: 27 gases (5 combined with 7.5 hours)

For PFP, even the very moderate 40-minute Gaussian filtering was skipped locally around the major leak in order to preserve the extraordinarily steep rise in concentration (see Figure 1, Figure 2, and Figure 10).

MAIN FINDINGS BY ANITA ON THE ISS

ANITA has measured several gases on the ISS that currently are not detected by other means (ammonia) or are not routinely measured by real-time or archival methods, including PFP and SF₆. In addition, many gases in the ISS air 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 and the number of crew members present, and the functioning of the air revitalisation systems. ANITA has given detailed time-resolved information on very different gases such as carbon monoxide, methane, ammonia, PFP, SF₆, siloxanes, alcohols, carbon dioxide, and water vapour [22]. An example on how much information may emerge from time-resolved information on just one single gas is given in the following.

ANITA's time-resolved PFP variations gave several new types of information:

- A. ANITA's observed PFP oscillations during fast carbon dioxide removal from the ISS air revealed previously unknown coupling between PFP and the US CDRA (Carbon Dioxide Removal Assembly) [22].
- B. An incidence on the ISS was suspected to indicate a PFP leak. This could be ruled out by ANITA's PFP data, limiting the search for the correct diagnosis of the incidence [22].
- C. A major leak of PFP from an ISS cooling system, and also a later service-related release, could be quantified and followed with high precision and high time resolution for significant time periods.
- D. The concentration details in item C over hours and days revealed that the PFP concentration was stabilised rather quickly, apparently after the PFP penetration into less accessible air volumes had been completed. It could therefore be concluded that neither the American nor the Russian attempts to clean the air of PFP were successful, so that the extra cleanup actions could be terminated. – The detailed dynamics of item A also helped to explain why the US CDRA failed to remove PFP from the ISS air.
- E. Owing to the stability of PFP in the ISS air, PFP can be exploited as a tracer gas to calculate the effective relative air volumes of any visiting spacecraft (not carrying PFP!) or new modules sharing cabin air with the ISS. In practice for the ANITA mission, these calculations were mainly used in the opposite direction in order to have an extra check on ANITA's reliability [22].

Since the major PFP releases to the ISS cabin air occurred after submission of ref. [22], details of the main leak are shown in Figure 1 and Figure 2 (for full overview see Figure 10).

As mentioned above, ammonia is currently not routinely measured in the ISS air, and no standard system for

time-resolved measurement is available. ANITA measured ammonia varying mostly between 0.10 and 0.15 ppm in the ISS cabin air, when a 5-day Gaussian filter was applied [22]. This absence of events implies a very important finding, viz. that there was no significant ammonia leak from the cooling systems. ANITA can measure and track the ammonia concentration far below the human odour threshold value. And ANITA's excellent precision allows the detection of even a very small ammonia leak that makes the air concentration rise slowly, even over days and weeks.

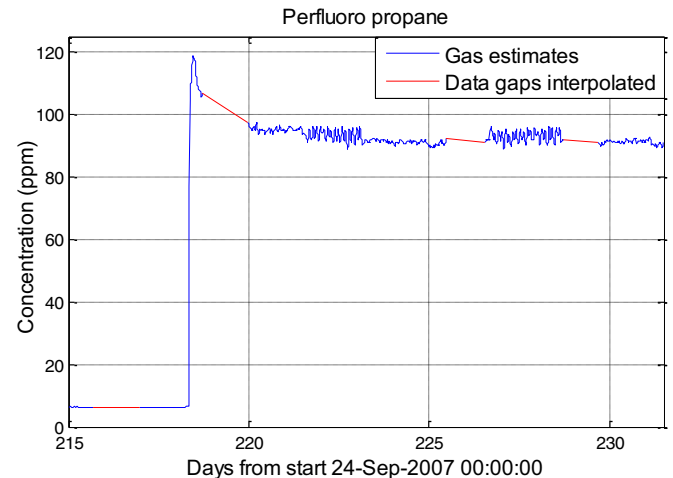


Figure 1. Overview of the main perfluoro propane leak event on April 29, 2008. The gas estimates have been filtered with a Gaussian filter (FWHM 40 minutes) except at the steep rise, where the original data estimates have been kept. The periods of time where the noise looks larger in reality exhibit regular oscillations induced by the US CDRA (see the text, esp. list item A, and [22]).

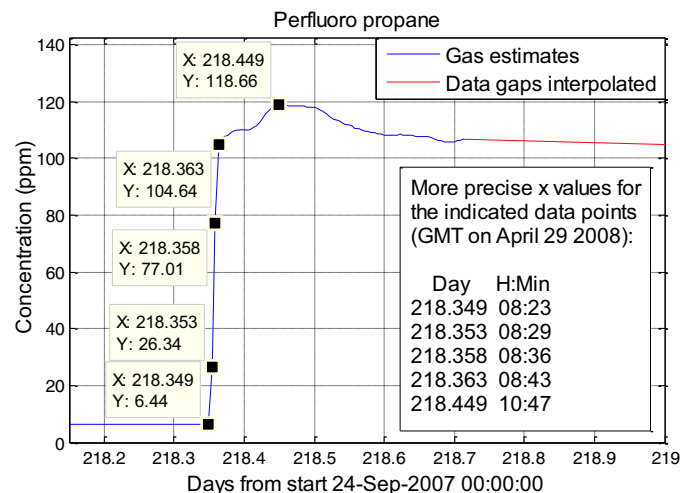


Figure 2. Details of the main perfluoro propane leak event on April 29, 2008. The gas estimates have been filtered with a short Gaussian filter (FWHM 40 minutes) except at the steep rise, where the original estimates have been kept.

COMPARISONS TO OTHER INFORMATION ON THE ISS AIR

BASIS FOR COMPARISONS

In general, and especially since ANITA is an experimental system, it is important to compare the results to other sources of information on the ISS air. Current operations utilize real-time monitors and archival samplers to achieve a complete picture of ISS air quality. The real-time monitors that target compounds in common with ANITA include the VOA (volatile organics), CSA-CP (CO), CDM (CO₂), and MCA (CO₂, methane). The archival samplers, grab sample containers (GSCs), are returned to ground for analysis by GC and GC/MS methods. The GSC analysis is considered the reference method for most compounds. Exceptions are siloxane compounds that have proven to be unstable in the GSCs.

Comparison of real-time data to ANITA results is somewhat limited because with the exception of the MCA, the other instruments were operated only periodically. The other instruments only had occasional analytical sessions that overlapped with ANITA operations; however trending from these devices can be used to achieve some perspective on the ANITA performance.

Eight grab samples collected in Destiny during the ANITA operations can be used for comparisons to ANITA. However, one special grab sample was taken directly in front of ANITA. This excellent source of data for comparison is specially emphasized below.

Grab samples represent snapshots in time, while ANITA data give a sequence of data points with six-minute or half-hour intervals (for onboard operation and standard downlinked spectra, respectively). This sequence of data is primarily intended for time resolution of the gas dynamics, but it has also been exploited for spectral sifting and time domain filtering in order to improve the noise level and detection limits of the gas estimates. For most gas compounds, this time averaging has a minimal effect on ANITA comparison to other methods, because the ISS air composition usually changes slowly, unless an event occurs or crew activities have a localized effect on the air. Exceptions include PFP and CO₂ [22], but even for these gases the fast variations only amount to a few per cent in concentration. Also, the filtering of ANITA's estimates is tentatively limited to preserve the significant variations (see above). In total, a few hours difference in air sampling is normally not significant, and anyway the comparison graphs may indicate if a time difference might be significant. Also, the ISS is a well-mixed atmosphere so that samples acquired anywhere in Destiny can confidently be used for comparison with ANITA results.

When we compare different air measurements, the sampling technique is a crucial element affecting sample

stability as well as potential losses. It should be noted that ANITA only holds air samples for a few minutes, so that all compounds that are stable in the cabin air on this time scale are stable in ANITA's air samples as well. The main potential problem is losses to the inner surfaces of the sampling system. However, any such losses are expected to be small, and they would tend to even out over time through saturation of absorption or adsorption on the surfaces, mostly causing memory effects and thereby slower reaction. For the reference measurements using grab sample containers (see below), these problems are potentially worse. However, testing has shown that the surface treatment of the GSCs and the sample handling in general successfully avoid errors for the target compounds.

As part of the evaluation, ANITA's results have been analysed and cross-tested in different ways in order to assess their reliability. Important information on significance has also been extracted from how the gas estimates reflect ISS events like spacecraft dockings and gas releases.

Owing to the special problems with spectral disturbances (ghosts) and line shape changes for ANITA on the ISS, it is highly interesting to find out whether such non-ideal influences in ANITA's optical spectra can have lead to significant errors for a given gas. The most probable error would be a concentration offset, and this type of error is difficult to identify from ANITA's concentration curves alone. Therefore other information must be exploited.

For highly stable gases like PFP and SF₆, checking for concentration offset is possible through calculation of air mixing ratios with visiting spacecraft.

In principle, it is also possible to look for the size of the spectral details of the gas in question. However, this is essentially an approach like classical spectral analysis for gas estimation, which is highly inferior to ANITA's calibration for multi-gas measurement. Therefore, direct spectral analysis to support ANITA results is difficult in general, and it is not feasible close to ANITA's detection limit for the target gas. For the ISS operations, the spectral disturbances add to the problems. Still, it has been possible to check for ANITA offset for two very interesting gases, viz. carbon monoxide and methane, as well as SF₆ and PFP under the following circumstances:

- The target gas concentration is clearly above ANITA's detection limit for averaged spectra
- The target gas exhibits a very distinctive spectral pattern
- For each measured IR spectrum, ANITA's gas estimates and procedure for calculation of the residual spectrum are applied to emphasize the spectral contribution of the target gas (subtracting the effects of all other known gases)
- Many spectra are averaged