Appendix II - Infrared Instruments (FTIRs)

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Infrared spectroscopy is an analytical technique with a long history in environmental science and chemistry. Very-high-resolution Fourier Transform Infrared Spectroscopy (FTIR) has supplanted other infrared techniques because of its superior performance. The FTIR technique has been widely used in atmospheric chemistry and has been validated by exercises such as the Balloon Intercomparison Campaign (BIC) and its use in the validation of space-based measurements such as for the Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment, MIPAS, MOPITT, SCIAMACHY, ACE, TES, HIRDLS and others is well documented. Thus, it has become one of the primary measurement techniques within NDACC. Low spectral resolution instruments are appropriate for total column data only, while high spectral resolution spectroscopy can also retrieve vertical profile information. The fundamental techniques are the same for both types of observations. Nevertheless, individual FTIR instruments, as well as other infrared instruments such as emission spectrometers, must still be validated. Such validation has been defined by the NDACC Infrared Working Group (IRWG) for both the retrieval of total column abundances and for the derivation of trace gas vertical profiles. However, some methods of calibration and validation are unique to each type. Emission instruments also have the potential for contributing to the suite of NDACC IR measurements.

Quality Criteria for the Evaluation of New Instruments and Instrument Teams

Details regarding the application for NDACC affiliation and the associated validation requirements in general are provided in the NDACC Measurements Protocol and the NDACC Validation Protocol respectively. The process for validating column measurements obtained using an FTIR instrument within NDACC is summarized in Figure 1. Validation is a multi-step process that may require some time to complete. Investigators proposing inclusion of their group and instrument into the NDACC / IRWG should observe the following guidelines. Further information regarding the NDACC and its Data, Measurement and Validation Protocols may be obtained at

http://www.ndacc.org/

and for the IRWG in particular at

http://www2.acom.ucar.edu/irwg/

Minimum Requirements for Instruments and Analysis Techniques

Observing site selection is an important factor in validation. An ideal site for stratospheric observation is at high elevation (to avoid as much tropospheric water vapor as possible) and away from urban centers (to avoid local emissions

and pollution). However, as the NDACC focus has broadened to include tropospheric source gas measurements, instruments at lower altitudes and closer to urban centers have become more acceptable and useful. A diversity of site characteristics and global coverage are considered important, and proposals from any site are welcome for submission to and review by the IRWG. Proximity to other NDACC instruments, which employ UV, microwave, or Lidar techniques, is also useful but such co-location of instruments is not essential.

Proposals to the IRWG should include detailed technical descriptions of the site, instruments, and analysis techniques.

New high-resolution instruments should meet the following minimum conditions:

1. Optical path difference (OPD): a minimum of 120 cm is acceptable; however, 250cm is recommended for high resolution instruments for optimal profile retrieval,
2. Spectral range: 1900-4100 cm-1 (minimum) (CaF2 beamsplitter), 700–5000 cm-1 optimum (KBr beamsplitter)
3. Continuous spectral coverage (except for the 6-7μm H2O region) in a small number (less than 8) of spectral (filter) bands,
4. Ability to record full-resolution spectrum (in one filter band) in approximately one minute,
5. Ability to make regular timely (sub diurnal) measurements on an ongoing basis (decadal).

For the total column measurements by low-resolution instruments, a minimum OPD of 1cm is acceptable (1). Bandpass filtering is not required (3), the other criteria listed above are required.

Since not all instruments may be able to fulfill all of these requirements, it is necessary for the Investigator to document instrument performance for review by the IRWG. High signal-to-noise ratio in the spectra is necessary for the detection of weak absorptions and for the retrieval of vertical profiles; however there are no set minimum requirements. If the proposed instrument is a commercial instrument of the same type as a previously accepted NDACC instrument, the description can be brief, referring to the accepted instrument and highlighting any differences. The IRWG (or a subcommittee thereof) will determine whether the instrument performance meets NDACC requirements.

A description of the Investigator's data analysis method must be supplied, along with the sources of any supporting data such as line parameters and constituent, temperature and pressure profiles. In particular, if the technique is not currently in use in the IRWG, some comparisons showing commensurate results must be provided. An ability to perform retrievals in accord with IRWG best practices and retrieval parameters must be shown.

Independent Evaluation of the Instrument Design and Data Analysis
Investigators interested in the IRWG validation process should consult the following documents at the NDACC/IRWG website: IRWG Inter-comparison

Summary, IRWG Uniform Retrieval Guidelines and IRWG Validation Strategy. A sub-committee of the IRWG or referee will be designated to review the application for new instruments or investigators. The process leading to certification of a team and instrument should consist of (but is not limited to) submission to the referee of:

- Solar absorption spectra taken by the instrument at the site,
- Retrievals of several of the required NDACC gases for total columns,
- Retrievals of several of the required NDACC gases for VMR profiles,
- Spectra of a low pressure gas cell e.g. HBr and N2O with derived column and ILS data,
- Spectra and retrievals taken in a blind intercomparison if available,
- Retrievals from other spectra submitted to them and
- Uncertainty estimates of derived columns and or profiles retrieved.

Test cases should be selected, which include gases with simple line structure (e.g. HF or HCl), with complex structure (e.g. HNO_3), and with a known column abundance (e.g. N_2 or CO_2). Species are to be selected from the list of primary archived IRWG gases. Constraints must be placed on the input temperature and pressure profiles (e.g. standard IRWG T-p profiles from NCEP should be employed), the shape of the mixing ratio profiles, and the freedom allowed in adjusting the volume mixing ratio in the fitting for a true comparison of instrument/retrieval performance.

Through this exchange, suggestions and recommendations may be relayed to the Investigator to improve the quality of the measurements and their analysis to conform to IRWG network best practices. During this time the investigator is welcome to attend IRWG meetings to discuss his/her progress.

Instrument and Data Analysis Intercomparison

Before performing comparisons of data retrieval procedures and the results of atmospheric spectra, laboratory measurements should be performed with cells containing low partial pressures of HBr or N_2O. The focus of the analysis of these measurements is on the retrieval of the instrumental line shape (ILS) parameters [Hase, 2012]. Further details and cell evaluation software can be obtained at the IRWG website. These parameters along with cell spectra should be forwarded to the referee. Data along with error analysis should be stored in the IRWG standard GEOMS HDF file format.

Acceptance Criteria for New Instruments

The referee or a designated subcommittee will examine the results of the intercomparison and make a recommendation to the IRWG. The recommendation will be based in part on the sensitivity of the instrument (random noise in the retrieved columns), the consistency of measurements between the evaluated and reference instruments, and the instrument performance with respect to instrument line shape, zero-level errors, phase errors, and line asymmetry.

Quality Criteria for the Evaluation of Continuing Instruments and Teams
The Investigator has primary responsibility for ensuring the quality of data from his/her instrument on a continuing basis, and for submitting the data to the NDACC Data Host Facility in a timely manner. He/she is also responsible for maintaining up-to-date documentation files describing the instrument and its quality control as outlined in the NDACC Measurements and Data Protocols.

Several formal tests are required periodically to ensure the data quality and the intercomparability of data from different sites, and to become fully validated for each species. Since it is impractical to bring together all of the FTIR instruments for repeated instrument intercomparisons, several methods have been adopted for continued data quality evaluation.

For those species (e.g., ozone, water) that are measured at an NDACC site by techniques other than FTIR, continuous intercomparison of retrieved columns (and profiles, as applicable) should be performed to maintain confidence in all of the techniques implemented at the site. IRWG members are encouraged to participate in cross instrument intercomparisons organized for this purpose. Opportunities for intercomparison with satellite measurements should be used, both for mutual evaluation and for enhancing the scientific output.

One or more mobile instruments that have been validated in intercomparison campaigns may be available for transport from site to site for side-by-side comparisons. Agreement of results from these instruments and the permanent site instruments will provide evidence for the validity of both measuring systems. In the case of disagreement, further experiments will be needed to determine the origin of the difficulties and optimize the measurements. For this reason, it is useful for two instruments to travel to a site for comparison with the fixed instrument. Results from all of these intercomparisons must be documented in the NDACC archive and publication is encouraged. Because of the difficulty and cost of such comparisons, they will be relatively infrequent, perhaps every three to five years at a given site.

Each site should have one or more optical cells. These cells should contain known amounts of the gases at low pressure for routine evaluation of instrument performance, especially the instrument line shape. The gases used should be linear molecules (for well-separated lines), heavy (for narrow Doppler widths), easy to handle (for convenience), and not present in large concentrations in the atmosphere (so that the cell can be used in the direct solar beam to evaluate the performance during actual data collection). The IRWG has adopted cells of HBr and N_2O constructed for this purpose. Specifications and/or cells can be obtained from the IRWG. These tests should be performed at least bi-monthly, and the results included in an archive at the instrument site. Provision for measuring the temperature of the gas in the cell during the operation should be available.

At each IRWG meeting a subset of these cells should be brought to the site for measurement on a common instrument. The column and ILS should be determined by the hosting group and another IRWG member. Results should be

archived at the IRWG web site.

If possible, monochromatic laser sources should be used to evaluate the instrument line shape. For further advice please see Griffith or Hase alignment procedures:

Griffith_alignment.pdf

and

HaseBlumenstockAlignment.pdf

Investigators should routinely analyze their data to obtain the column abundances of gases with known concentrations such as CO_2, N_2, and O_2, whenever possible. These data should be reported along with the other trace gas columns obtained [Barthlott et al., 2015]. The FTIR columns should be compared regularly with the column amounts determined by other NDACC instruments at the same site where there are common species and the measurements are comparable.

There should be an ongoing exchange of spectra and analysis results among the various infrared groups. This will help prevent systematic differences in the analysis methods and provide early detection of any data quality problems that may develop. A careful, defensible, and consistent way of assessing the random and systematic uncertainties in the retrieved columns must be developed by the IRWG. Retrieval comparisons within the IRWG are ongoing and may be more or less formal. Groups are strongly encouraged to participate and take actions based on accepted improvements that result from the comparison.

It is anticipated that the processes of data collection and analysis will become more and more automated in the future. It is the Investigator's responsibility to ensure that all data archived are examined in such a way that high data quality is maintained and that undetected errors do not enter by the automation process.

Changes in Instruments and Data Analysis

Since one of the major goals of the NDACC is the detection of long-term trends, care must be taken in any modifications of the instrument or data analysis, which could affect the results. Once the regular operation of an instrument has begun, such changes should not be undertaken lightly; consultation with the IRWG is recommended. The primary data (interferograms) should be retained by the investigator indefinitely so that improved data processing or retrieval techniques, including improved spectral line parameters, can be applied retrospectively to the earlier data. In such cases, the entire dataset should be reprocessed and archived, along with (at least) reference to earlier versions.

If/when an instrument is replaced, an overlap of measurements should be undertaken if at all possible to determine whether any artifacts from the transition exist in the derived data products that have been previously archived. If this is not possible, other means of certifying the new instrument as outlined

above may be undertaken.

Instrument Intercomparisons

The NDACC Instrument Intercomparisons Protocol provides a general description of the methods recommended for formal impartial instrument intercomparisons leading to the validation and certification of instruments for use at NDACC stations. The following details address issues associated with the formal intercomparison of high spectral resolution infrared instruments but are also viable for low-resolution instruments.

It is recognized that the difficulties associated with moving large delicate instruments may limit the opportunities for multiple instrument intercomparisons. Hence, such opportunities should be planned carefully by the IRWG to maximize their usefulness and to minimize their cost. If one or more traveling instruments have been compared successfully with several accepted instruments, the latter can subsequently serve as transfer standards. Provisional acceptance of an instrument may be recommended by the IRWG while awaiting finalization of logistical arrangements for the formal intercomparison.

If possible, the intercomparison should be conducted at the actual NDACC site where the FTIR operates. In any event, the range of solar zenith angles employed should correspond to observations at the target site(s). Observations should be made on at least five clear days and spectra should be analyzed for no less than five of the primary NDACC molecules and N_2. Sufficient observing time should be used to ensure that random noise does not limit the retrievals substantially. Spectra should cover the entire observable spectral range. Measurements by the instrument being evaluated and the reference instrument should be made coincident in time to the extent practical. Agreed upon profiles of temperature, of pressure, and of the constituent to be scaled should be used in the analysis. Standard retrieval parameters currently accepted and in use by the IRWG, such as spectral fitting regions, line parameters, and *a priori* data should be used for the analysis.

As discussed in the Instrument Intercomparisons Protocol, quick-look data should be submitted to the referee after the first day of the intercomparison. The referee may advise the participants of any major problems, in order to optimize the time of the intercomparison. Following a brief troubleshooting period based on the referee's advice, the comparison will become blind until its conclusion.

The analysis should provide the derived vertical column amount and profile for each of the target gases from the entire day's spectra and the estimated random and systematic uncertainties in the columns and profiles. Any additional derived results, such as the instrument resolution or modulation efficiency and phase error, should also be documented. Spectra encompassing the fitted regions used in the analysis should be provided, along with the residuals from the fits. As with all formal intercomparisons, the results should be submitted to the referee within one month of the completion of data collection, prior to learning

the results from other instruments.

References

F. Hase, “Improved instrumental line shape monitoring for the ground-based, high-resolution FTIR spectrometers of the network for the detection of atmospheric composition change,” Atmospheric Measurement Techniques, vol. 5, no. 3, pp. 603–610, doi:10.5194/amt-5-603-2012, 2012.

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Figure 1. NDSC IRWG Path to Validation