EURAMET
European Association of National Metrology Institutes

Title: Spectral reference data for atmospheric monitoring

Abstract

Spectro-analytical techniques are indispensable for atmospheric remote sensing. The target species spectrum is the key dataset for such instruments and serves as an inherent transfer standard. These spectra could enable traceability in atmospheric measurements if they were measured in a traceable fashion, but this is rare. There is evidence that observations of some atmospheric species, key to understanding climate change, may be inaccurate by 10's of percent. Metrology is required in order to address these issues so that the accuracy of data from the global networks of monitoring stations over the last 2-3 decades are fully characterised and future measurements are enabled at uncertainties of <10 %. This will facilitate the development and testing of improved atmospheric models that will in turn provide the improved climate change predictions required by policymakers.

Conformity with the Work Programme

This Call for JRPs conforms to the EMRP 2008, section on "*Grand Challenges"* related to *Environment* on page 24.

Keywords

Spectroscopy, spectroscopic data, atmospheric measurements, satellite and airborne sensors, climate change, HITRAN, IPCC, NDACC, FTIR spectroscopy

Background to the Metrological Challenges

Monitoring climate change without chemical remote and in situ sensing of the atmosphere is as hard to envisage as is atmospheric remote sensing without spectroscopic measurement techniques. The quality, accuracy and traceability of such diagnostic techniques completely depend on the traceability of the spectroscopic data, i.e. the molecular spectra of the target species and their dependence on pressure, temperature and composition of the matrix.

The large atmospheric range and variability of pressure and temperature within the troposphere and stratosphere, the large spatial heterogeneity down to the metre scale, e.g. in clouds or in layered atmospheres, and the strong optical disturbances e.g. by particles/droplets, all lead to significant problems with the correction of the matrix effects in atmospheric remote sensing.

Climate model validation often requires the accurate detection of very small changes on large background signals while traceability is absolutely essential in order to ensure comparability over the long time scales necessary to detect climatic changes and over the large range of instruments in use. Both applications require high sensitivity, traceable measurements, for which highest quality spectral data of the target signatures and the most important perturbers over the full range of atmospheric boundary conditions are indispensable.

The HITRAN [1] and GEISA [2] databases are two of the best-known and most extensive resources containing several million line strengths of tens of molecules. The model reference spectra produced from these databases underpin much of the global atmospheric measurement effort, hence they directly influence the quality of qualitative and quantitative analysis. However, whilst they have been put together with great expertise and have served the community well, atmospheric quantifications carried out using these invaluable tools are undermined due to a number of metrological issues. This is exemplified by a study done with the SCIAMACHY instrument onboard ESA's ENVISAT satellite. Unexpectedly large tropical emissions of methane were observed [3]. Recently however, a retrieval error was identified related to inaccuracies in water vapour spectroscopic parameters, causing an overestimation by 30 % of methane correlated with high water vapour abundances [4]. A further example demonstrating the requirement for improved characterization of uncertainties and established traceability of such measurements is the need to reconcile differences between remote sensing techniques and in-situ measurements (*e.g.* based on chemical analysis).

These issues are attributable not just to the databases but the overall measurement process. A key example of this is in ground-based upward looking FTIR measurements of the atmosphere made from monitoring stations scattered across the globe. These stations have been monitoring key atmospheric species over the last 2-3 decades in order to provide important trend data to understand changes occurring in the composition of the atmosphere and also for the validation of models used in predicting future climate trends. Side-by-side comparisons between a transfer standard and instruments permanently installed at these stations have shown that in some cases uncertainties in quantification of stratospheric and green house gases may be in the order of 14.3 % HNO_3, 9.7 % HCl, 7.7 % HF, or 6.4 % N_2O [5]. Which is unacceptable considering that, N_2O which not only regulates stratospheric ozone but is also a green-house gas with 298-times greater impact per unit weight than carbon dioxide.

The project proposals addressing these challenges may be considered as a part of a wider, longer-term European spectrometric infrastructure to be developed, which is capable of determining and disseminating traceable spectroscopic gas phase signatures of environmentally important molecules to significantly improve spectroscopic atmospheric measurements on all measurement platforms as well as for global sensor networks.

Scientific and Technological Objectives

Proposers should address the objectives stated below, which are based on the PRT submissions. Proposers may identify amendments to the objectives or choose to address a subset of them, in order to maximise the overall impact, or address budgetary or scientific / technical constraints, but the reasons for this should be clearly stated in the JRP-protocol.

The following objectives exceed the budgetary scope and time frame of a typical JRP. The proposers shall prioritise accordingly, considering opportunities in later EMRP calls. The proposers shall describe how and on the basis of what stakeholder input they prioritise the species under consideration.

The JRP shall aim at:

1. Production of traceable, high resolution spectroscopic data of all key atmospheric species, i.e.:
    a. Line positions and their pressure dependence
    b. Line strengths and temperature dependence
    c. Line width and shape and dependence on pressure, temperature and collision partners

All parameters need to be recorded across the range of physical conditions relevant to the various atmospheric layers to enable a traceable validation of the major databases of spectroscopic parameters

2. development/setup of a holistic spectrometric infrastructure for traceable spectral line data, including:
    a. spectroscopic hardware and data retrieval software
    b. improved Fourier transform infrared (FT-IR) or tuneable laser spectrometers, and
    c. measurement cells for the above-mentioned purposes
    d. reference gas mixture preparation (static / dynamic)
3. development of traceable spectroscopic measurement /data evaluation strategies, i.e. including complete GUM based uncertainty calculations, e.g. characterisation of the uncertainties associated with the instrumental line shape functions in FT-IR spectrometers used in global atmospheric monitoring networks

The proposers shall describe the detailed mechanisms by which the data will be made available to the stakeholders.

Proposers shall give priority to work that meets documented stakeholder needs and may include measures to facilitate the development of European standards and Directives.

Proposers should establish the current state of the art, and explain how their proposed project goes beyond this.

Potential Impact

Proposals must demonstrate adequate and appropriate participation/links to the “end user” community. This may be through the inclusion of unfunded JRP partners or collaborators, or by including links to industrial/policy advisory committees, standards committees or other bodies. Evidence of support from the “end user” community (eg letters of support) is encouraged.

Where a European Directive is referenced in the proposal, the relevant paragraphs of the Directive identifying the need for the project should be quoted and referenced. It is not sufficient to quote the entire Directive per se as the rationale for the metrology need. Proposals must also clearly link the identified need in the Directive with the expected outputs from the project.

You should also detail other Impacts of your proposed JRP as detailed in the document “Guidance for writing a JRP”

You should detail how your JRP results are going to:

- feed into the development of urgent standards through appropriate standards bodies
- transfer knowledge to the atmospheric monitoring community.

You should also detail how your approach to realising the objectives will further the aim of the EMRP to develop a coherent approach at the European level in the field of metrology. Specifically the opportunities for:

- improvement of the efficiency of use of available resources to better meet metrological needs and to assure the traceability of national standards
- the metrology capacity of Member States and countries associated with the Seventh Framework Programme whose metrology programmes are at an early stage of development to be increased
- outside researchers & research organisations other than NMIs and DIs to be involved in the work

Time-scale

The project should be of 3 years duration.

Additional information

The references were provided by PRT submitters; proposers should therefore establish the relevance of any references.

[1] L.S. Rothman, *et al.,* JQSRT, 110 (2009) 533.

[2] N. Jacquinet-Husson, *et al.,* JQSRT, 109 (2008) 1043.

[3] C. Frankenberg, J.F. Meirink, M. van Weele, U. Platt, T. Wagner, Science, 308 (2005) 1010.

[4] C. Frankenberg, *et al*., Geophys. Res. Lett., 35 (2008) L15811.

[5] C. Paton Walsh, W. Bell, T. Gardiner, N. Swann, P. Woods, J. Notholt, H. Schütt, B. Galle, W. Arlander and J. Mellqvist, J. Geophys. Res., 102 (1997) 8867.