NDACC Theory and Analysis Protocol

Introduction

The Network for the Detection of Atmospheric Composition Change, NDACC, aims to encourage the widest possible use of its data. The role of the Theory and Analysis Principal Investigators (PIs) is to enhance awareness of this NDACC data and to encourage and facilitate its exploitation. Subject to the Protocol for Data Providers and Data Users, interested scientists may have direct access to all data products.

The analysis and verification process through which atmospheric observations are transformed into NDACC data involves collaboration between the experimental measurement and modeling scientists. Such collaboration is valuable in areas such as: (i) data analysis (both the forward model and the retrieval of geophysical parameters), (ii) statistical studies to ascertain the significance of the results, (iii) application of atmospheric modeling for the validation of the data, and (iv) scientific analysis of the data. This document provides information on both general and specific needs of the Instrument Working Groups (IWGs) and suggests areas of potential collaboration. Scientists interested in collaborating with the IWGs are encouraged to contact the PIs of the relevant instrument(s) as well as the Theory and Analysis Working Group Representatives on the NDACC Steering Committee.

General Needs of the Instrument Working Groups

Sampling Plans

Sampling plans must be designed to account for the general needs of the NDACC programs as well as the specific requirements for detecting changes in a given species measured by an instrument at a chosen site. These plans are required for all measurements to enable the early detection of trends in species or parameters with the required sensitivity, while not overburdening operational resources. Aspects of experimental design, such as measurement frequency, need to be constructed from a statistical point of view, with attention given to parameter or species variability (e.g., sampling and testing standard deviations), autocorrelation in successive values, measurement locations, missing values, averaging periods, coincidental measures of other species, etc.

Quality Assurance and Control Plan

Guidelines for quality assurance and control are needed by the instrument PIs to maintain instrumental accuracy and precision at the highest levels possible. These guidelines should have a strong basis in statistical quality control that includes regular calibration checks and the detection of special cause variation (e.g., instrument drifts, inadequate viewing conditions, etc.). Experimental design procedures need to be applied to identify controllable operating conditions that keep the instruments on target with minimal measurement (i.e., analytical) variation. Control charts are needed for evaluation of instrument performance against a set of standards.

Intercomparison Activities

NDACC measurements from different instruments need to be compared for consistency and for identifying statistically significant differences. Intercomparisons with measurements obtained from satellite instruments are critical. The interpretation of significant measurement differences between instruments measuring the same parameter requires collaboration among instrumental, theoretical, retrieval, and/or statistical scientists.

Error Analysis

Error analysis and retrieval characterization need to be made in a unified and comparable manner, so that the nature of the remote measurements can be properly understood and intercomparisons can be carried out correctly.

Analysis of Long-Term Variability and Trends

Statistical analysis of NDACC data can include time series analysis of observations, along with more sophisticated comparisons to state-of-the-art chemistry-climate model (CCM) and chemistry transport model (CTM) simulations. Time series analysis can involve multivariate regression studies to identify trends and other variability linked to the effects of the QBO, ENSO, solar cycle and other factors. Detailed comparisons with simulations could include quantifying variability of temperatures and numerous trace species across a range of spatial and temporal scales, providing comprehensive fingerprints for validating model behavior and interpreting the long-term NDACC observations.

Specific Instrument Working Group Needs

Collaborators who bring experience and expertise in the following areas could make a very valuable contribution to NDACC activities.

Lidar

Retrieval Techniques - In all cases lidar signals have to be processed to obtain range resolved values of the geophysical parameters of interest (e.g., ozone or water vapor concentrations, temperature, and aerosol scattering ratios). This processing generally implies spatial filtering, temporal averaging, and range derivative of the raw signals. Various methods have been developed using different filtering techniques (polynomial, derivative filters, windowing, etc.) to adapt the range resolution of the measurements to the expected signal to noise ratio. In particular, the range resolution has to vary with altitude. This will allow the determination of the real altitude resolution and precision of the measurements. In addition, the magnitude of various systematic errors related to the use of ancillary data (ozone cross-section dependence on temperature, influence of pressure boundary conditions on temperature retrievals, calibration of aerosol measurements, etc.) should be studied further.

Microwave

Spectroscopy - Microwave retrievals can only be as good as the forward radiative transfer models used in the inversion process. The accuracy of the forward models depends mainly on the line list and the spectral line parameters used in these models.

Theory and analysis collaborators could include experts in microwave spectroscopy who could interface with the PIs to ensure that forward model line lists are kept current.

Retrieval Theory – While retrievals based on optimal estimation theory are now standard for NDACC microwave groups, proper characterization of fundamental retrieval properties such as vertical resolution and errors remains an important area of study. Advice and critical questions on these topics from experts in retrieval theory are always welcomed.

Atmospheric Temperature - Ground-based microwave measurements make use of background temperatures in their retrievals. Currently, this is generally obtained from local NCEP (or sometimes ECMWF) analyses in the stratosphere, and is supplemented by MLS measurements (in some cases an MLS climatology) in the mesosphere. There has, to our knowledge, been no systematic study of the long-term stability of the NCEP temperature analyses at NDACC stations. Such a study, based upon comparisons between the NCEP analyses and local balloon measurements would be useful in identifying possible drifts and discontinuities in the NCEP data, or in any other analysis or reanalysis, provided for NDACC sites on the NDACC website. This study would be aided by detailed knowledge of changes in the satellite measurements assimilated into the model. Hopefully such a study would produce a bias-adjusted temperature product that could be used by many NDACC measurements.

Exploitation of Unique Microwave Capabilities – A unique capability of the NDACC ground-based microwave instruments is to provide nearly continuous (24-hour/day) measurements of middle atmospheric profiles from a single location. In the case of the ozone measurements it is often possible to provide useful retrievals of stratospheric ozone over timescales of hours. Any advice on the application of such high temporal resolution measurements over long periods would be welcomed.

<u>UV/Visible Spectroscopy</u>

UV/Visible observations of chemical species are carried out largely during twilight conditions and, therefore, require a good understanding of twilight chemistry. In addition, understanding the air mass factors characterizing the vertical columns of species measured requires a detailed analysis of scattering processes. Spectroscopy in the 300-700 nm region is a key aspect of the data analysis including consideration of the Ring effect, polarization, and the effects of clouds. Finally, as with other measurement techniques, a thorough understanding of error analysis is needed to aid in the NDACC data analysis and verification process.

<u>FTIR Spectroscopy</u>

The Infrared Working Group (IRWG) measures column amounts and vertical profiles of many stratospheric and tropospheric species using infrared spectroscopy and remote sensing profile retrieval techniques. Solar viewing, high resolution instrumentation is required to provide long term records of ten primary species: O_3, $ClONO_2$, HCl, HF, N_2O, CO, CH_4, C_2H_6, HCN, HNO_3. Investigations of other species are also routinely performed. These data provide the ability to measure decadal trends, seasonal and diurnal cycles and anomalous events. The IRWG also pursues data products from other moderate- or low-resolution solar instruments, emission IR spectrometers, and from short term airborne, balloon borne or ground based campaign instruments. These latter instruments may have attributes that differ from the high resolution instruments at permanent stations, such as better vertical resolution (balloon), isolated stratospheric columns (airborne), high time resolution and high local density observing (low spectral resolution), or continuous operation (emission).

The analysis of these data requires model calculations to understand the underlying processes, to distinguish between chemically and dynamically induced changes, and to better characterize the observed air mass by providing data of additional species and meteorological data such as equivalent latitude. Studies using IRWG data from multiple stations require global chemistry models. Models using tagged tracers, including back trajectory models, are especially useful for detailed analyses of emissions and their impacts. In some cases these studies may be augmented with regional models.

Model support would also be advantageous for understanding the climatology and variability of proposed measurement sites.

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