NOVAC technical meeting

4 – 8 February 2019
Gothenburg, Sweden

Notes of the meeting

Objective:

Presenting current status of NOVAC software and hardware and taking decisions on implementations and publications for 2019.

Participants:

Chalmers (hosts): Bo Galle and Santiago Arellano

VDAP/USGS (co-organizers): Christoph Kern and Diana Norgaard

Heidelberg U.: Ulrich Platt and Florian Dinger

Collaborators: Mattias Johansson (software), Manne Kihlman (hardware), Joakim Möller (database)

Invited but not possible to attend: Claudia Rivera (UNAM), Nicole Bobrowski (Heidelberg U.), Silvana Hidalgo (IGEPN), and Zoraida Chacón (SGC)

Organizers:

Christoph Kern (USGS/VDAP), Bo Galle and Santiago Arellano (Chalmers)

Location and local contact:

Chalmers University of Technology, Dep. Space, Earth and Environment, Hörsalsvägen 11, Floor 4

Summary

The NOVAC technical meeting served to level off the knowledge of different groups on the present status of the hardware, software and data analysis developments during the last months, as well as to discuss future actions and publications related to the network. Unfortunately, due to several reasons, not all members of the Steering Committee were able to attend the meeting; however, all important conclusions are summarized in the following.

Hardware:

Following discussions after the NOVAC meeting in Peru, Manne presented a proposal for replacement of the MOXA computer, which will not be commercialized in the future, and instrument electronics (see Hardware WG report, June 2018). During this meeting, Manne presented the result of its implementations, which can be summarized as follows:

Computer and electronics:

- Computer: Axiomtek model IFB122-FL-DC, 0.84 W, 1 USB, 2 Serial, 2 ETH, industrial-standard, 4 GB disk
- Spectrometer: support previous models of OceanOptics (using serial for communication and USB for power) and Avantes USB2048-ULS series (using USB2/3 for communication and external 12V power source). Avantes spectrometer consumption is 4.2 W in idle mode and 4.8 W in acquisition mode.
- USB port is expanded through a hub to connect spectrometer (power to OceanOptics, communication for Avantes) and GPS (GlobalSat)
- Serial port is connected to a module to control one (optionally two) stepper motor, as well as a thermometer and voltmeter.
- Stepper motor driver allow micro-stepping, making scanning much smoother.
- Configuration of the computer is done through ETH or basic configuration through Serial.
- All components are commercially available and can be integrated without expertise. A user manual is available, in principle minor soldering of serial module components and installation of the kongo program is all what is needed to assemble the new instrument electronics.

The new computer/electronics has been tested independently by Chalmers and a demonstration was done during the meeting.

The changes were done having in mind: (i) compatibility to older versions of the instrument (in principle an old computer and electronics can be replaced by the new one, only changing the PS/2 GPS receiver by a USB GPS receiver); (ii) robustness to environmental conditions; and, (iii) easy integration without expertise.

The last criterion follows from the decision of Manne of not continuing with mass-producing the electronics in the future and to facilitate replacements by the users.

Spectrometer:

A basic comparison of signal-to-noise based on parallel skylight measurements was conducted to compare the standard spectrometer OceanOptics S2000 to an OceanOptics USB2000+, an OceanOptics Maya2000

Pro, and an Avantes USB2048-ULS. The first two are essentially the same spectrometers, and the last two have back-thinned UV detectors. Unfortunately, the Avantes spectrometers that were available for test did not have the exact characteristics that would be needed for the NOVAC instruments, so the comparisons were not conclusive.

Based on experience on colleagues and manufacturers descriptions, the most interesting alternatives to the S2000 (out of production) are the OceanOptics Flame and the Avantes USB2048-ULS with back-thinned detector.

Both the new version of the kongo software and the MobileDOAS program recognize and run acquisitions with all OceanOptics and Avantes spectrometers that were available, including a Flame (borrowed for communication tests only, since optical characteristics were different).

Kongo software:

Manne presented a new version of the kongo software to run on Axiomtek and handle also the Avantes spectrometer. This last requirement was facilitated due to availability of drivers for RaspberryPi, which use the same type of processor than the Axiomtek, and which were kindly provided by the local distributor of Avantes. To communicate with an Avantes spectrometer, the user should specify the parameter SPECTROMETERTYPE=AVANTES in the cfg.txt file inside the computer.

During summer last year, two new functions were added to kongo:

- 'cfgmain.txt': this is a new 'master' configuration file that includes a list (in absolute or relative paths) of configuration files for different types of measurements. For example, it could contain ten entries of the standard, scanning 'cfg.txt' file, followed by one entry of a 'cfgwind.txt' file to run dual-beam wind measurements, and then another entry for a 'cfgfixed.txt' file to run fixed-direction measurements at a different angle. If only standard scanning measurements are needed, the user could obviate cfgmain.txt and only include the standard cfg.txt file as in the past. The names of these files are arbitrary, except that at least one should be named cfg.txt.
- 'MINELEVANGLE': this is a new parameter in the configuration file that corresponds to the angle (in degrees) of the solar elevation at which the scanner is activated. For example, if a value of 20 is selected, the computer will calculate the solar position based on information of the GPS and activate the scanner only if the sun is above 20 degrees on both horizons. If the scanner is in the middle of a measurement and the elevation angle reaches the threshold, the measurement is finalized and then the scanner stopped smoothly. This function can be used together with the 'Sleep function' of the NovacProgram and with a physical timer, but it provides more autonomy to save power in the instrument without requiring connection with the observatory or if the timer is not available.

During the meeting it was requested that only one version of kongo (handling different types of computers and spectrometers) exist and that the number of bits of the spectrometers (defining the scales of possible intensity values) be recognized. These changes were implemented during the week by Manne.

Future actions:

- Find more robust, field-proof USB modules for the new computer
- Design a box to house the computer and electronics with simple and robust connectors to all peripherals (GPS, motor cable, power cable, and spectrometer). The Gothenburg company building the scanner may be consulted for this task
- Acquire a OceanOptics Flame and an Avantes with required characteristics for further tests of performance and compatibility

Software:

Mattias and Diana presented the status and discuss around the most important issues with the MobileDOAS and NovacProgram software, which are listed in the GitHub platform, and which have been subject of work during the last months.

Some additional issues were identified and described as new items for further work, while a few other were disregarded because they were considered unnecessary or already solved.

A general principle that they will try to follow is harmonizing as much as possible all common functions used by the three programs (both mentioned above and the NOVACP3, used for batch-processing). This will facilitate implementation of changes and simplify the codes. When it comes to the implementation of new functions, the general principle will be to do it first in the batch-program, where it can be tested before its implementation in the other, instrument-oriented, programs.

There is also a compilation of the NOVACP3 for the Ubuntu distribution of Linux. This has been tested for a limited set of data in a virtual-machine environment, where it ran correctly, but more tests are required. The goal is to run this software in the computer cluster of Chalmers in a pseudo-automatic way, to produce re-analysis of flux data for the observatories. The Linux version created by Mattias skips the user interface and requires functionalities found in the open-source POCO C++ library.

Discussions were focused on categorizing the priority of each of the items in GitHub. A new requirement was to create a tool to simplify the generation of wavelength calibration files and convoluted reference cross sections for the spectrometers. This tool may then implement more sophisticated methods to retrieve the instrumental function and calibration from measured spectra (see below).

The general structure of the NOVACProgram was explained to Florian for planning on how to implement several algorithms developed in Heidelberg over the last years.

Diana and Mattias attended several sessions where data analysis algorithms were discussed, but tried to use some hours for hands-on work on the several issues, with a focus on the MobileDOAS software.

Christoph outlined the mDOAS software (based on MatLab) that he developed and which is used by USGS to process data from traverses. Some features could be used by the MobileDOAS software, in particular handling of external meteorological data and more advanced estimation of uncertainties.

Bo suggested to implement a visualization tool in the NovacProgram to identify and plot measurements in single-direction/wide-field-of-view mode, to plot time-series of slant column densities at different time window (see more below).

A summary of specific issues and its priority for implementation is given below:

- BrO/SO2
    1. One ratio per scan
    2. Sophisticated way to find daily statistics
- Lineshape
    1. Implement convolution tool (calibration and lineshape)
    2. Implement Gaussian fit of Fraunhofer lines (on measured spectrum)
    3. Ídem, but for super-Gaussian
    4. Validate and implement the tool in NovacProgram
- Scattering
    1. Implement convolution tool and matrix inversion (DOAS type)
    2. Implement a way to get best estimate of VCD from PDF
    3. Implement as post-analysis tool in MobileDOAS/NovacProgram
- Wind forecast
    1. Ability to read netCDF
    2. Ability to extract relevant level from best information on plume height
- Single-direction measurements
    1. Recognize that measurement is of this type
    2. Plot column vs. time
    3. Possibility to look beyond current-day
- Bugs/additions:
    - Data with different UTC date in the same day, is plotted as if it would have the same date
    - Time series plot shows 'Local time', but it should be 'UTC time'
    - Implement 'history tab' to be able to look for flux data for a period of time (look for source code of NovacViewer)
    - Update instrumental manual with latest changes (GitHub)

Data analysis:

Several aspect of data evaluation were presented and discussed during the week, as summarized below:

Wind data:

Santiago presented the status of the retrieval of wind data for flux evaluations of NOVAC data. The best product available was the new ERA5 re-analysis database from ECMWF. This provides the result of model data constrained by observations with global coverage, with a model spatial resolution of about 36 km and a time resolution of 1 h. The data is retrieved with a Python code which prepares a request that is queued for running in the servers of ECMWF. We presently retrieve wind vectors, relative humidity and cloud cover with an interpolation of 0.25 deg/1 h and 22 pressure levels from ground to about 10 km altitude. This data is retrieved in netCDF format and saved in a local computer or ftp server. The files are then converted to formats legible by the NOVAC software (txt or wxml) after further spatial interpolation to the coordinates of each volcano's summit.

The best strategy would be to modify the NOVAC software to be able to read netCDF directly and make the necessary interpolations as well as to automatize the routine to save re-analysis and forecast data in the server, as it was implemented in the past for wxml files.

BrO/SO2

Florian presented the general routine used to obtain time series of molar ratios of BrO/SO2 and a plan for implementation of BrO SCD retrievals from NOVAC data. The proposal consists of three 'levels' of data, from the selection of useful data for further retrieval, through the binning of data (spectrally or statistically), to the actual computation of daily BrO/SO2 molar ratios. The present algorithms developed in Heidelber run on DOASIS (jscript), and the idea is to migrate them into C++, in order to make them part of the NOVAC software. A first step will be to implement it in the batch-processing software and subsequently in the NovacProgram.

Retrieval of instrumental function

Ulrich and Florian presented the concept and some results of the retrieval of instrumental function of the spectrometer from measured skylight spectra, fitting a 'super-Gaussian' function to selected Fraunhofer lines. These functions allow in principle to adjust asymmetric curves of various shapes (peaked or flattened), depending on the number of parameters (2 to 4), and could be applied to different spectral regions to account for possible variations in the instrument function with wavelength. The method has been published (Beirle et al., AMT, 2017) and Ulrich has made contact with a colleague (Borger) at Mainz who could be willing to share code for its implementation. Florian presented results of analysis of the variation of lineshape with temperature and over time, obtained from a similar retrieval on actual NOVAC data. The results are consistent with laboratory experiments done by BIRA at the beginning of the project. It was suggested that each new spectrometer is subject to temperature variation tests before installation, but this would be lengthy. It was decided that we should try to implement the retrieval of instrumental function and calibration using a symmetric super-Gaussian or a simple Gaussian as a first step. The batch program and observatory software allow today for adjustment of the wavelength calibration using the Fraunhofer lines, but not lineshape.

Synthetic Fraunhofer spectrum

Florian presented a summary of the algorithm to derive absolute SCDs using a synthetic background (Fraunhofer) spectrum and its application to data from Nevado del Ruiz (published by Lübcke et al., AMT, 2016). The method requires some training data, and achieved a worst limit of detection than the standard use of a measured background spectrum used in NOVAC, but it would be interesting to use it as a diagnostic tool to detect possible 'contamination' of the background spectrum by volcanic gas. Another alternative is to use a measured 'clean' spectrum from a different time as a reference, also to check for contamination. It is not considered a priority for implementation at present.

Radiative transfer

Ulrich presented results of the MSc work of Katja Bigge (manuscript in prep.) on several radiative transfer effects on the flux calculations of simulated NOVAC-type measurements using the Monte-Carlo code MCARTIM. They show that contamination of background spectra can be more problematic than previously thought, as well as the effect of the position of the sun respect to the scanning plane. Both overestimation and underestimation is possible, but the maximum errors were below 30% for the cases studied.

Christoph presented results of the inversion of extremely high SCD from mobile-DOAS measurements of the plume of Kilauea. The extreme opacity of the plume caused considerable attenuation of the light intensity, which is used to estimate a range of aerosol optical depths in the plume, using MCARTIM. The method uses a Markov-Chain Monte Carlo approach to characterize the knowledge of possible values of entry variables (aerosol optical depth, vertical column density, aerosol extinction coefficient) based on the measured spectra and then runs radiative transfer simulations to update that information and obtain statistical distributions of the variables. The evaluations are done in the 'long wavelength' range of SO2 absorption.

Santiago presented the status of recent work at Chalmers to obtain better estimates of the straight-path column densities, which are required for the flux calculations in NOVAC. The method evolved from a 'sky subtraction' algorithm at adjacent bands of different absorption strength (presented by Bo in Costa Rica, 2015), to a more general retrieval of the distribution of possible optical paths, by extending the plume transmittance factor into a series and solving the problem in matrix form. The algorithm is of simple implementation and fast and it has been proved with synthetic data, data generated with MCARTIM and measured data in traverses. From the distribution some work is needed to determine the straight-path, and some ideas of what would be needed for this were discussed during the meeting, including generating more data using MCARTIM.

Single-Direction measurements with wide-field-of-view optics

Bo presented some results of the use of this measurement strategy in Iceland and PNG. The method uses a cylindrical lens attached to the prism of a flat scanningDOAS to obtain an elongated field of view in one direction and the narrow field of view in the transversal direction. By aiming the scanner in direction of the plume it is possible to integrate optically the entire plume and obtain fast measurements of the flux under favorable conditions. The method is more apt for situations where null or weak emission exists, for example to detect anomalous emissions from a quiet volcano. Christoph presented results of laboratory experiments and analysis that showed that the method could get accurate flux estimates if the column densities are low and if the intensity homogeneous within the field of view. This last requirement is not met in the present system, affecting accuracy, but the strategy may still be used as an early-warning.

Since the method could be interesting for measurements in more volcanoes, it was requested to add functionalities in the NovacProgram to detect and visualize these measurements (SCD vs. time) at different time windows. Such a functionality exists already as a separate python code (used e.g. by IMO).

Infrastructure and resources:

Data repository

Joakim was invited for a discussion around the repository of daily flux data from NOVAC, which his company MolFlow developed last year, and which was presented during the meeting in Peru. The present website hosting this data repository is not active, but could be activated at any moment. The website allows exploring available raw data and data with useful flux calculations and to visualize and download data resulting from the batch-processing done at Chalmers. Only statistics of daily emission are presently

included, and the data can be downloaded in netCDF and ASCII formats, after a simple registration procedure.

The present plan is to make this data repository public after submitting the 'flux compilation' article and confirming consent of the observatories. Only data for the period March 2005-January 2017 will be made public.

During 2019 the plan is to implement an automatic routine to post-process the data and send back evaluated results to the observatories. This data could then be made public with a certain grace period or kept for exclusive use of the observatories. The procedure will be discussed with the observatories later this year.

The best way to disseminate data from this repository to other databases such as WOVOdat, EarthChem, ECCAD or Smithsonian would be by implementing and API (application programming interface) in the repository, although the effort will be justified only if data is going to be shared in the future.

Data server

Chalmers hosts a server, which was acquired about ten years ago, for centralized back-up of the data obtained by NOVAC stations operated by the observatories. This data is further copied in servers hosted at Heidelberg and Brussels. The server has required replacement of some components and service by Chalmers IT personal. There is a need to acquire a new server.

The login credentials to this server are easily accessible (in fact, it can be googled!). There were several discussions about the urgent need to improve the security of this server. One approach is not to include the default credentials in the NovacProgram, but rather assign credentials to each observatory. This should be done during a transition period of a few months, the best would be to agree on teleconferences with each observatory to implement the changes. Another action is to encrypt the server communication.

It was also discussed the vulnerability of having only one centralized server, since data from the observatories cannot be re-routed in case of a failure of this server. Although switching of servers is a possible solution, it seems difficult to implement in the short term.

Mirror data servers

It is understood that both Heidelberg and Brussels keep mirroring the server at Chalmers, but not entirely confirmed. At least the group at Heidelberg is actively using an independent download of the data, but they think the original server is still active.

Resources

Chalmers has the possibility to keep working on NOVAC topics in the middle term, due to recent extension of Santiago's position to 2+2 years based on a grant from the Swedish space agency. This means, in particular, the possibility to keep administrating and hosting the data server, to keep assembling instruments, and to keep working on data analysis. Main focus of the grant is to work on satellite data, and the ambition is to combine NOVAC data with TROPOMI and implement an automatic routine to feedback evaluated data to the observatories. During the rest of 2019, Bo will use funding from Chalmers to continue developments in hardware (i.e., new spectrometer and computer), software (i.e., batch program and updates of the mobileDOAS and NovacProgram) and the data repository (i.e., developing and hosting the database).

VDAP keeps strong involvement in NOVAC and will maintain 25% of the work of Diana, as well as assembly and installation of instruments. They have some resources to finance short visits for specific work, e.g., on software or training. Plans for a next NOVAC workshop were not discussed in specific, but it will most likely be organized in 2021. USGS is expected in strengthen cooperation with universities in the US and the National Academy of Sciences will launch a program for 'middle-scale infrastructure' that could open possibilities for NOVAC involvement.

Heidelberg has not succeed in securing funding in the previous year for work related to NOVAC, but they have ambitions to continue the work and apply again for funding this year. The new director (succeeding Uli) will most likely not keep working on volcanic emissions, and most of current graduate students are strongly linked to activities at the Mainz MPIC, especially in satellite research. However, several developments (BrO evaluations, lineshape retrieval, Fabry-Pérot cameras) will be important to keep and expand through the NOVAC platform. Florian goal is to defend his thesis after summer and look for an academic position to maintain his work on the analysis and interpretation of volcanic gas emission data. Plans to involve a Fraunhofer institute in long-term work with NOVAC had not been successful so far, due to complicated politics.

Publications:

Flux compilation 2005-2016

Santiago discussed briefly the ambition to present a manuscript of the evaluation of the dataset 2005-2016 for all volcanoes in NOVAC, which was presented in discussed during the meeting in Peru. All observatories were requested to provide feedback on the data, but only few have replied. Data in the manuscript is intended to be made public through the NOVAC daily flux repository (presented in Peru). The manuscript is drafted but not finished. Chalmers aims for finalizing it during March 2019.

Radiative transfer

After further tests agreed during the meeting, the plan is to prepare a publication summarizing the 'sum-over-optical-paths' method and its implementation to mobileDOAS and scanDOAS measurements. The goal is to have a first draft before summer 2019.

Review for JVGR

Christoph has been invited to write a review article on remote sensing of volcanic plumes and solicited input from other participants. The journal is JVGR and therefore the scope would have to have a strong component of 'volcanological' use of the data, rather than more technical aspects. Some ideas were discussed, the deadline is not defined, but it will most likely not be ready before the first half of this year.

Other:

Uli presented a seminar to members of the Microwave and Optical Remote Sensing division at Chalmers about an overview of DOAS remote sensing of atmospheric composition and several new applications, which was very well attended.