Ensuring High-Quality Data from NOAA’s GC-MS PERSEUS Instrument

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Introduction
A new gas chromatography-mass spectrometry (GC-MS) analytical system for Preconcentration of Environmentally Relevant Species (or PERSEUS) was completed in October 2014 (Pic. 1, 2 and Fig. 2). Since October 2014, almost 27,000 discrete air samples have been measured on PERSEUS for:
- 10+ hydrocarbons (e.g., ethane, propane, benzene)
- 35+ halocarbons (e.g., CFCs, HCFCs, HFCs, PFCs)
- 3 sulfur-containing compounds (e.g., OCS, SF6, SO2)
- For temperatures, data are also collected via stripcharts.

Data Quality Assurance

- Instrument long-term reproducibility
- System nonlinearities
- Inter-laboratory comparisons
- Sample storage tests
- Leak identification - collection
- Blank corrections
- Contamination - collection
- Peak identification
- Co-located samples

Summary and Conclusions
- Data from NOAA/ESRL/GMD’s air sampling networks are vital to large-scale studies of halocarbons and hydrocarbons.
- To be most effective, these long-term data records must be carefully scrutinized so samples with collection or measurement problems are identified.
- Quality assurance and quality control (QA/QC) are performed with different methods and programs developed at GMD and SIO. This includes:
  - Monitoring sample water vapor content, system diagnostics, and system nonlinearities.
  - Comparing results from independent measurement systems and different sampling methods.
  - Conducting routine tests of equipment and routine analyses of archive tank air.

Remaining Issues and Future Plans
- Assign uncertainties for reported PERSEUS analytes.
- Apply corrections to PERSEUS analytes affected by nonlinearity.
- Convert to new tagging software for sample collection process (CCGG samples only).
- Continue to compare results with independent measurement labs.
- Continue to learn about the instrument as we perform more tests.

Data Quality Control

- Stripschats
  - 24 diagnostic traces are stored in the form of a stripchart for every sample analyzed. Fig. 3 shows a stripchart with irregular T1 temperatures, potentially causing poor results for samples with early eluting analytes.

- Blank corrections
  - Blanks are run twice per day and all measurements are corrected based on an interpolation between blanks (Fig. 4).

- Contamination - collection
  - Toluene contamination from new materials in the PFP pumping units is shown in Fig. 7.

- Unexplained measurement problems
  - Fig. 5 shows lab air contamination of HFC-152a standards when canned spray products are used near the measurement lab.

- Peak identification
  - Fig. 11 shows the peak identification process for CH3Br. Real air from NWR (top) is compared to a synthetic mixture of pure CH3Br in zero air (middle) to verify that we get the same analyte spectra. This allows us to choose the most abundant ion that doesn’t show coelution in real samples. We also compare to the NIST spectra (bottom).

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