

**Guidance for EPA Supersites Investigators
For Data Reporting Conventions for
Level of Data including Temperature and Pressure Conditions,
Units, and Below Detection Limit Data
From the Quality Assurance Working Group**

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The EPA Supersites Program's Quality Assurance Working Group provided the following guidance to Supersites Program Principal Investigators (PIs) on certain conventions to follow when reporting data to the NARSTO Quality Systems Science Center for archiving. This guidance is in addition to guidance provided by the Data Management Working Group on matters such as formatting data in the Data Exchange Standard and following the consensus metadata standards for site names, variable names, and flags.

1. Level of data to report, including temperature and pressure conditions.

Mass/volume measurements (e.g., from filters) should be reported as concentrations, rather than separately as mass and volume. PM mass data should be referenced to local ambient temperature and pressure conditions to be comparable to federal reference method PM data. Associated meteorological data should be reported either in the same file or in a referenced meteorological data file as described below.

Gas flow, volumetric measurements, and mass/volume conversions, must be reported at known (ambient or standardized) temperature and pressure conditions. The associated temperature and pressure conditions should be provided in the same file, or these should be available from file(s) of meteorological data from the same site or closest available site. If these are provided in the same file the temperature and pressure measurements should be available at the same time basis as the measurements. However, if temperature and pressure measurements are available less frequently than the target measurement, only those values actually measured should be presented in the data file. Missing value codes (not interpolated values) should be used for times when no actual measurements of temperature and pressure were taken.

If measurements are standardized, EPA prefers that the reference conditions, i.e., 298.15°K (25.00° C) and 760 Torr (760 mm Hg); be used as stated in Section 40 chapter 50.3 of the Code of Federal Regulations. Whatever temperature and pressure conditions are used they must be documented in the Data Exchange Standard's *TABLE COLUMN VOLUME STANDARDIZATION Key Phrase.

2. Units

Chemical variables and particles - Please use the following guidance about units for chemical variables and particles:

- Typically particles are reported in mass/volume units, varying depending on the levels: ug/m3, ng/m3, pg/m3, etc;
- Gas phase species are typically reported in units of ppm, ppb and ppt by volume;
- Organic compounds in the gas phase are to be reported as ppmC, ppbC, or pptC by volume;
- Fog or cloud measurements are typically reported in units of microequivalents per liter or micromoles

- per liter. Please avoid using mass/volume for these kinds of measurements;
- It is difficult to come up with a single unit for all chemical species, and we allow variation due to convention;
- Conversion factors may be used to achieve these conventional units;¹
- We provide a table of standard non-chemical variable names, with strongly recommended units. These are SI units in most cases. Please use these units (with appropriate prefixes), or consult with the Supersites Data Management Working Group if there is a compelling reason to use different units.

3. Representing below detection limit data.

If a measured value is below what is considered to be the normal “Detection Limit” (DL) but is nonetheless considered, meaningful, suggesting where between zero and the DL the value lies, the measured value should be provided, and the NARSTO V2 flag (“Valid estimated value”), should be applied. If an investigator’s detailed flags are being used one or more of these may also be applied.

If the value is an average with some or all the values in the average below the DL and the data are still meaningful, the value should nonetheless be provided, in part because it may be statistically useful, and the NARSTO V1 flag (“Valid value but comprised wholly or partially of below-detection limit data”) should be applied. One or more detailed, “study” or “network” flags, also may be used.

Consensus metadata standard for flags can be seen at the following Internet Web site address:
<http://cdiac.esd.ornl.gov/programs/NARSTO/metadatastandards>.

It is recommended that (1) uncertainty estimates be provided with each measurement in the dataset (see separate guidance about representing uncertainty), and (2) that DL values be reported either as a table in the associated detailed metadata documentation or in the data file. If uncertainty estimates, such as precision and bias, cannot be provided with each measurement, they should be described in the detailed metadata documentation (again, see separate guidance about representing uncertainty).

While we encourage investigators to report all measurements, including values below the DL, we discourage data censoring through data substitution such as the use of a constant value, i.e. the DL, 50% DL, or zero. If a constant value is reported, it should be flagged with the new NARSTO V7 flag (“V7: Valid value but set equal to the detection limit because the measured value was below the DL”). The detection limit value substituted should be defined in the metadata file.

4. Applying MDL Flags

Condition	Flag
Value is below the DL but the value is considered meaningful	V2
Value is in an average and part or all of the data in the average are below the DL however the value is considered a meaningful estimate	V1 or V7 (see below)
a) actual measured value is provided	V1

b) substituted value equal to the DL value is provided	V7
c) substituted value equal to a constant (e.g., 50%DL or zero DL)	This practice is discouraged for research data

Example 1: Reporting below-DL values without substitution

Value	Flag	Notes (these are NOT the flag definitions)
5.32	V0	Valid
3.49	V0	Valid
0.05	V0	<i>Valid (this measured value is at the Detection Limit)</i>
0.04	V2	Valid, below DL but considered quantifiable, meaningful, or usable
0.03	V2	Valid, below DL but considered quantifiable or meaningful, or usable
0.02	V2	Valid, below DL but considered quantifiable or meaningful, or usable
0.01	V1	Valid, below DL and Principal Investigator lacks confidence in it, but may be statistically useful
-0.01	V1	Valid, below MDL and Principal Investigator lacks confidence in it, but may be statistically useful
-0.02	V1	Valid, below MDL and Principal Investigator lacks confidence in it, but may be statistically useful

Example 2: Reporting below-DL value with substitution

Value	Flag	Notes (these are NOT the flag definitions)
5.32	V0	Valid
3.49	V0	Valid
0.05	V0	<i>Valid (this measured value is at the Detection Limit)</i>
0.04	V2	Valid, below DL but considered quantifiable or meaningful
0.03	V2	Valid, below DL but considered quantifiable or meaningful
0.02	V2	Valid, below DL but considered quantifiable or meaningful
0.05	V7	Valid, the measurement was below DL and the Principal Investigator lacks confidence in it and the DL was substituted in its place.

5. Background and Acknowledgments

Initial Drafts of this material were prepared by S. W. Christensen, based on Quality Assurance Working Group and Data Management Working Group calls. Section 2 was modified from material contributed by Paul Solomon. Section 3 reflects extensive early comments and augmentation by Bill Sukloff, Bob Vet, and Les Hook. Sections 1 and 3 reflect additional comments by Jeff West, Dennis Mikel, and Paul Solomon with further modification after discussion on the July 3 data management working group call. Guidance on reporting uncertainty is a related topic, but this is being treated in a separate document.

6. Reference:

1. Finlayson-Pitts, B.J. and Pitts, Jr., J.N., 1986. Atmospheric Chemistry. John Wiley & Sons, New York.