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GML Quality Manual for Measurement Services

Main Document

Approved by

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1.0 Introduction and Scope

The provision of measurement services, which includes calibration services and certified reference materials, is an element of the work carried out by the Global Monitoring Laboratory (GML) of the Earth System Research Laboratory, National Oceanic and Atmospheric Administration (NOAA) in support of its Central Calibration Laboratory (CCL) roles within the World Meteorological Organization Global Atmosphere Watch (WMO/GAW) program. Our goal is to provide services essential to the operation of WMO/GAW contributing measurement programs for greenhouse gases (GHG) and other related tracers.

GML has served as a Central Calibration Laboratory of WMO/GAW for CO₂ since 1995, and for several other greenhouse gases at later dates (see <http://www.esrl.noaa.gov/GML/ccl/>). GML has championed the use of high-quality reference gases (reference materials) for many years, and has strived to ensure that GML measurements and those within WMO/GAW are linked to traceable, reliable reference materials that are internationally accepted. A commitment to quality lies at the heart of long-term records produced by GML, and extends to GML CCL roles. The international standard ISO/IEC 17025 and relevant requirements of ISO 17034 specify the general requirements for the competence to carry out tests and/or calibrations and characterize reference materials. It is GML policy to conform to ISO/IEC 17025 and ISO 17034 to the extent allowed by statute and regulation, considering also the needs of WMO/GAW partners. Requirements of ISO 17025 and ISO 17034 are both addressed in this document and sub-level documents.

The GML Quality Manual (QM) describes GML policies and procedures related to the objectives described herein. Details for each calibration service (CO₂, CH₄, CO, N₂O, SF₆), the preparation of compressed gas standard mixtures (reference materials), and the primary standards upon which calibrations are based are documented as Technical Procedures (Table 1).

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Table 1: List of sub-level documents

| Document Name | Subject | Type |
|------------------------|---|---------------------|
| TP_primary_manometer | manometric primary standards (CO ₂) | technical procedure |
| TP_primary_gravimetry | gravimetric primary standards | technical procedure |
| TP_analysis_CO2 | CO ₂ analysis | technical procedure |
| TP_analysis_CH4 | CH ₄ analysis | technical procedure |
| TP_analysis_N2O | N ₂ O analysis | technical procedure |
| TP_analysis_SF6 | SF ₆ analysis | technical procedure |
| TP_analysis_CO | CO analysis | technical procedure |
| TP_reference_materials | reference materials | technical procedure |
| CCL_Personnel.xlsx | personnel responsibilities | |

2.0 Informative references

[Federal Information Security Management Act \(FISMA\) 2002](#);
see <http://csrc.nist.gov/groups/SMA/fisma/overview.html>

GAW Report No. 213: 17th WMO/IAEA meeting of experts on carbon dioxide, other greenhouse gases and related tracers measurement techniques, (Beijing, China, 10-13 June 2013), Geneva, Switzerland, 2014. https://library.wmo.int/pmb_ged/gaw_213_en.pdf

GAW Report No. 229: 18th WMO/IAEA meeting of experts on carbon dioxide, other greenhouse gases and related tracers measurement techniques, (La Jolla, CA, 13-17 September 2015), Geneva, Switzerland, 2016. https://www.wmo.int/pages/prog/arep/gaw/documents/FINAL_GAW_REPORT_229.pdf

19th WMO/IAEA Meeting on Carbon Dioxide, Other Greenhouse Gases and Related Measurement Techniques (GGMT-2017), Dübendorf, Switzerland, 27-31 August 2017, World Meteorological Organization, Global Atmosphere Watch Report Series No. 242, available at https://library.wmo.int/doc_num.php?explnum_id=5456

GML CCL Website: <http://www.esrl.noaa.gov/GML/ccl/>

ISO/IEC 17025:2017 General requirements for the competence of testing and calibration laboratories

ISO 17034:2016 General requirements for competence of reference material producers.

ISO Guide 31:2015 Reference materials – Contents of certificates, labels, and accompanying documentation

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JCGM 100:2008, Evaluation of Measurement Data – Guide to the Expression of Uncertainty in Measurement (ISO GUM 1995 with minor corrections), Joint Committee for Guides in Metrology (2008); http://www.bipm.org/utis/common/documents/jcgm/JCGM_100_2008_E.pdf

JCGM 200:2012, International vocabulary of metrology — Basic and general concepts and associated terms (VIM), JCGM 200:2012 (JCGM 200:2008 with minor corrections).

Letter of Agreement and Annex to the Letter of Agreement between WMO and NOAA/ESRL/GML, signed 23 April 2010.

Mutual Recognition Arrangement – Mutual recognition of national measurement standards and calibration and measurement certificates issued by national metrology institutes, Comité International des Poids et Mesures (CIPM) Paris, 14 October 1999, www.bipm.org/utis/en/pdf/mra.pdf.

Standards of Ethical Conduct for Employees of the Executive Branch, available at [https://oge.gov/Web/oge.nsf/0/076ABBBFC3B026A785257F14006929A2/\\$FILE/SOC%20as%20of%2081%20FR%2081641%20FINAL.pdf](https://oge.gov/Web/oge.nsf/0/076ABBBFC3B026A785257F14006929A2/$FILE/SOC%20as%20of%2081%20FR%2081641%20FINAL.pdf)

3.0 Terms and definitions

analyst: In analytical chemistry, an analyst is one who performs an analysis or a given part of a chemical measurement process; when used in the GML quality manual this term refers to a GML technical staff member qualified to perform a specific measurement process or part thereof.

calibration: Operation that, under specified conditions, in a first step, establishes a relation between the quantity values and corresponding indications (each with measurement uncertainties) and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication. (JCGM 200:2012, 2.39)

certified reference material: A reference material characterized by a metrologically valid procedure for one or more specified properties, accompanied by a certificate that provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability. (ISO 17034:2016, 3.2)

control standard: Any standard or material used to monitor the performance of a calibration system. A control standard could be a well-characterized gas sample (for gas analysis), or a well characterized object (for mass determination).

certificate: A document produced by GML to report the measurement results and uncertainties associated with analytical services and GML-supplied reference materials related to GML's function as a WMO Central Calibration Laboratory.

complaint: Any expression of dissatisfaction or concern made to an organization by, or on behalf of, an individual client – including government agencies – group or member of the public, related to the organization's products or services, or the complaints handling process itself.

ELOG: An electronic record keeping system used to record information pertaining to the

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operation and maintenance of analytical systems, software updates, and customer feedback.

gas standard: A cylinder of compressed gas (gas mixture) with mole fractions determined by primary means (see primary standard), or by analytical comparison to higher-level standards. For the purposes of this QM, all reference materials are gas standards.

GGMT: WMO/IAEA Meeting on Carbon Dioxide, Other Greenhouse Gases and Related Measurement Techniques. This acronym refers to meetings that occur every 2 years, organized by the World Meteorological Organization Global Atmosphere Watch (WMO/GAW). These meetings focus on technical aspects of measurement and calibration and are central to the planning and operation of WMO/GAW Central Facilities, such as Central Calibration Laboratories. For the purposes of this quality manual, the term GGMT community refers to an ad-hoc group of WMO/GAW scientists.

GML server: GML internal data access or data storage services that include capabilities for access control and archiving of GML documents.

GML method: For the purposes of this QM, a GML method is one that is documented in a technical procedure and validated by acceptable methods.

group chief: The highest ranking manager/scientist designated by the Director in the specialized research groups of GML.

management: A general term to describe the GML management levels above Technical Lead, specifically group chief and director.

measurement: Process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity. (JCGM 200:2012, 2.1)

measurement uncertainty: Non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used. (JCGM 200:2012, 2.26)

metrological traceability: Property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty. (JCGM 200:2012, 2.41)

primary standard: A measurement standard established using a primary reference measurement procedure, or created as an artifact, chosen by convention. (JCGM 200:2012, 5.4)

project coordinator (PC): A GML staff member with responsibility for tracking a calibration or reference material project from start to finish. The PC is responsible for communicating requirements to the appropriate analysts. The PC is the primary customer contact. A deputy PC may be designated.

quality management system, or management system: The organizational structure, responsibilities, procedures, and processes for implementing quality throughout the laboratory, and documented in the Quality Manual.

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reference material: A material, sufficiently homogeneous and stable with reference to specified properties, which has been established to be fit for its intended use in a measurement or in examination of nominal properties. (JCGM 200:2012, 5.13)

sales fixed fee memorandum of understanding (SFF MOU): An agreement between GML and a customer in which terms and conditions relating to calibration services or reference materials are defined.

target mole fraction: A fixed goal for the mole fraction of a particular component in a reference material.

technical procedure (TP): A compilation of steps or actions associated with a specific task.

technical lead (TL): GML member responsible for overseeing the technical aspects of calibration measurement or reference materials. GML staff may assume multiple roles (TL, PC, analyst).

valid range: The mole fraction range for which the method is valid (typically defined as the WMO/GAW scale range). The method may, in fact, be valid outside the specified range, but the extended validity may not be extensively documented.

4.0 General Requirements

4.1 Impartiality

NOAA/ESRL's Global Monitoring Laboratory of the National Oceanic and Atmospheric Administration conducts sustained observations and research related to source and sink strengths, trends and global distributions of atmospheric constituents that influence climate, contribute to depletion of the global ozone layer, and affect baseline air quality.

The measurements are of the highest quality possible, and document global changes in key atmospheric species. Research programs in key regions, utilizing an array of platforms including aircraft, balloons, ocean vessels and towers, complement the land-based information.

GML is committed to providing a workplace that is free of undue commercial, financial, and other internal and external pressures that would adversely affect the fit-for purpose quality of the technical work of the Laboratory. High standards of ethical conduct, impartiality, and objectivity are vital to the success of GML programs and required of all employees. Specific legal requirements and administrative guidance are provided to all employees in the publication Standards of Ethical Conduct for Employees of the Executive Branch.

4.1 Confidentiality

GML will inform the customer of information it intends to place in the public domain. Except that which is deemed publicly available by the customer, all other information considered

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proprietary shall be regarded as confidential. Calibration results will be made available on the GML web site, identified by cylinder number. No non-public customer information will be displayed on the GML website without customer consent.

Information related to customer complaints shall be deemed confidential, including the source, and shall not be shared unless agreed by the source.

5.0 Structural requirements

5.1 GML research

GML conducts research related to three broad themes:

- Tracking greenhouse gases and understanding carbon cycle feedbacks
- Monitoring and understanding changes in surface radiation, clouds, and aerosols
- Guiding the recovery of stratospheric ozone

Preeminent performance in these programs will allow realization of GML's Mission

"The mission of NOAA's Global Monitoring Laboratory has always been to provide high-quality, long-term records of atmospheric composition in a manner that allows the causes of change to be understood."- GML Research Plan 2018-2022

5.2 Laboratory management

The GML director is ultimately responsible for the quality of GML calibration services. This responsibility is delegated to group chiefs and technical leads directly involved in providing measurement services. The GML director is responsible for final approval of the top-level document, GML-QM, upon recommendation from technical leads and group chiefs involved in measurement services. Authority for approval of sub-level documents is delegated to group chiefs.

5.3 Scope of measurement services

The quality management system described in this manual covers measurement services (calibration and reference materials) provided to customers within WMO/GAW programs in accordance with GML's role as a designated institute of the WMO. Services described in this manual and supporting documents are limited to the functions of the Central Calibration Laboratories, and pertain only to calibration and reference materials for CO₂, CH₄, CO, N₂O, and SF₆, and only over mole fraction ranges corresponding to WMO scales (see, for example, GAW Report No. 242).

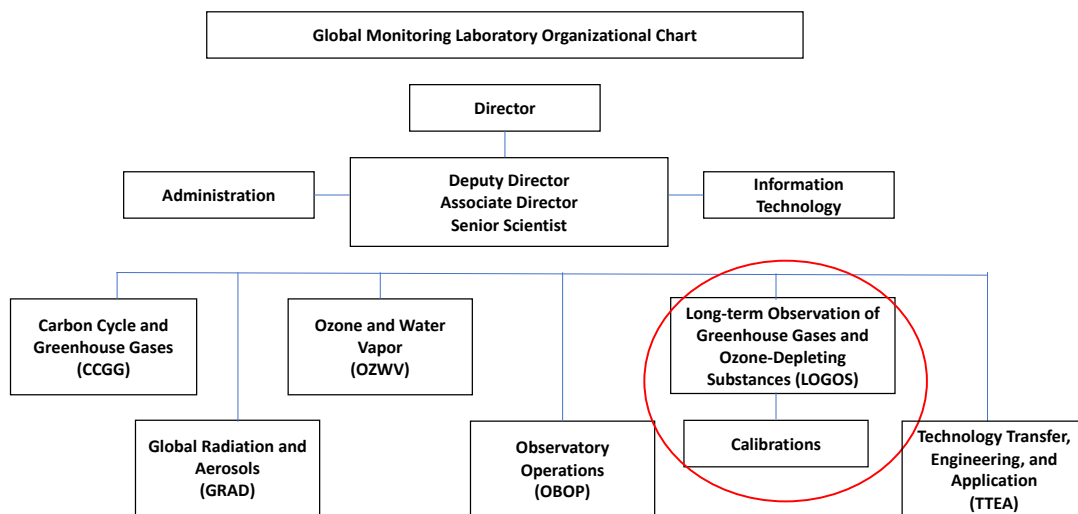
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5.4. Physical location

Relevant laboratories are housed within the David Skaggs Research Center building, at physical address 325 Broadway, Boulder, CO. Most reference materials are prepared at a field site in the Colorado mountains (named C1), through collaboration with the University of Colorado Mountain Research Station.

5.5 Organization chart

The Global Monitoring Laboratory is part of the NOAA Earth System Research Laboratories, and part of the Oceanic and Atmospheric Research (OAR) line office of NOAA. Other line offices within NOAA are the National Weather Service (NWS), NOAA Marine Fisheries Service (NMFS), National Ocean Service (NOS), NOAA Marine and Aviation Operations (OMAO), and National Environmental Satellite, Data, and Information Service (NESDIS). Calibration and measurement services described in this document are limited to activities within GML.



5.6 Responsibilities, authorities, and delegations

Overall authorities and responsibilities are delegated as follows: Analysts are responsible for technical aspects relating to analysis, and reporting results to the database. Technical leads are responsible for the integrity of calibration scales. Project coordinators are responsible for coordinating projects (agreements) and following projects through to completion. Analysts and

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technical leads have authority to gather information and make determinations related to instrument performance and data quality. Significant procedural changes should not be made without discussion among analysts and technical leads. Procedural changes that lead to changes in Technical Procedures should be approved at the group chief level.

6.0 Resource requirements

6.1 General

GML is committed to serving as a Central Calibration Laboratory in support of WMO/GAW. GML will support these efforts to the best of its ability, subject to the availability of funds.

6.2 Personnel

An updated personnel list is located on the GML server (//vnx4/CCL). Personnel performing tasks related to the preparation and analysis of reference materials are deemed qualified based on GML hiring and personnel evaluation procedures. Personnel hired through the University of Colorado, Cooperative Institute for Research in Environmental Sciences (CIRES), must possess a university degree as per CIRES policy. CIRES policy on hiring for research positions is determined by the Vice Chancellor for Research and Dean of the Graduate School (<https://cires.colorado.edu/about/bylaws>). Non-federal, non-CIRES contractors generally will not assist in the actual production of standards, but may be needed in an ancillary support.

Decisions for hiring and level of experience required are made at the group chief level, with input from additional staff. Training normally takes the form of mentoring, involving technical leads and analysts. Additional training needs or requests (goals) may be brought to the attention of technical leads and discussed at the group chief level. Records of employee responsibilities, training, and authorization, are maintained on a GML server. To aid in succession planning, each analyst should be trained on the operation of at least one other instrument. Training associated with safe laboratory practices is recorded at the Laboratory level for all GML staff members on an individual basis. It is the technical lead's responsibility to ensure that personnel performing work on CCL activities are competent.

Yearly evaluations of the performance of personnel involved in the production of reference materials will be conducted through the annual performance management cycle. Records of competence and performance are kept with employee personnel files.

6.3 Facilities and environmental conditions

6.3.1 GML, in collaboration with the General Services Administration (GSA), is responsible for assuring that environmental conditions do not adversely affect the quality of measurement services. Critical environmental conditions (i.e., those that could adversely affect measurement

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results if varied from those required) and the procedures for preventing them from compromising the quality of results are detailed in the Technical Procedures. The analyst determines whether requisite environmental conditions are met for a specific calibration service. Any stoppage due to environmental conditions should be documented in project records.

6.3.2 GML analysts monitor environmental conditions and their impact on analytical results. System performance is routinely verified using control standards, standards with a history of measurement, or by other means, and these data can be used to examine the effects of environmental conditions.

6.3.3 Measurement equipment is installed and operated in ways that prevent interferences between electronics. This includes segregation, as needed, from activities that are outside the scope of this manual. Chemicals and other laboratory consumables are stored under the conditions necessary to maintain their stability or integrity and to prevent cross-contamination with other materials.

6.3.4 Access to GML laboratories is controlled by key access for staff. GML follows site-wide policies related to safety and security for visitors and guests. Access to GML laboratories, offices, and storage areas is limited to GML personnel, authorized guests, security, safety, and housekeeping staff. No others may have access without the knowledge of the person responsible for the laboratory, office, or storage area. If necessary to ensure proper system performance and quality, access to certain GML laboratories may be restricted during certain periods. Use of critical equipment may be restricted as necessary, with management approval.

6.3.5 GML maintains a good working relationship with the University of Colorado, Mountain Research Station, within which the C1 facility for preparing reference materials is located. We have had a presence at the C1 site since the mid-1980s. It is the reference material technical lead's responsibility to ensure that this facility or an alternate facility meets the needs of GML with respect to its role as CCL.

6.4 Equipment

Equipment used by GML to prepare primary standards or analyze reference materials is used not only for services described in this QM, but also for internal work critical to GML's mission. Instruments used for value-assignment are identified by an instrument code, which is recorded in the database along with the measurement result. Test equipment or devices that influence certified values must have a calibration schedule and be properly maintained. If a calibration schedule is not recommended by the manufacturer, it is left to the technical lead to determine the calibration schedule. The schedule should be based on observed (or estimated) rates of change and the effect that these changes have on the results. Between calibration periods, function checks should be performed to ensure that the equipment is performing properly (see Technical Procedures). If there is evidence that a piece of critical equipment is not performing properly, the TL should be notified. Calibrations that depend on that piece of equipment should be postponed

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until the problem is fixed. Calibration programs and efforts to verify performance are documented in technical procedures. Records of calibration, maintenance, malfunction, and repair are logged in an electronic log (ELOG). The operator can usually determine if instruments are calibrated properly by examining historical records and/or analyzing test samples.

6.5 Metrological traceability

6.5.1 Routine calibrations are performed using instruments designed for this purpose. These instruments are traceable, through an unbroken chain of comparisons, to GML primary standards prepared by gravimetric or manometric methods.

6.5.2 Traceability of equipment used to prepare primary standards is established through an unbroken chain of comparisons, traceable to SI quantities temperature, mass, length, pressure, and amount of substance fraction (i.e. O₂ in N₂) traceable to NIST, either through calibration by NIST, or through an accredited facility.

6.5.3 In some cases, direct SI traceability may not be possible necessitating indirect or best-available links (see Technical Procedures). One example is isotopic ratios of stable isotopes of CO₂, knowledge of which are needed to establish calibration of the CO₂ analytical system. Here, traceability is established to secondary institutions with known links to internationally recognized primary reference materials. The contribution to uncertainty in the reference materials stemming from this secondary link is negligible.

6.6 Externally provided products and services

GML relies on externally provided services for the calibration of some equipment (e.g., temperature probes, analytical balances, pressure transducers). Schedules for routine calibration should be included in the Technical Procedures. Records of external calibrations will be kept.

Materials needed to prepare reference materials are also obtained from external suppliers. GML carefully evaluates materials (such as gas cylinders and compressed gases) for suitability. Specifications for critical materials, such as gas cylinders, shall be recorded and provided to suppliers.

7.0 Process requirements

7.1 Review of requests and tenders

All external requests for measurement services offered by GML are governed by policies specified in the Memorandum of Understanding (MOU). A Sales Fixed Fee (SFF) MOU is established between GML and the customer. The SFF MOU is reviewed annually by GML staff and at five-year intervals at higher levels of NOAA. Internal customers are handled via a web-based scheduling program, and do not involve an MOU.

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7.1.1 The procedure for creating and implementing a request for reference materials or calibration follows:

1. Customer makes initial contact through a GML ticket management system.
2. A project coordinator (PC) works with the customer to determine customer needs. The PC may supply the customer with a quotation.
3. The PC initiates a Memorandum of Understanding (MOU) for review and signature by the customer and NOAA. The customer sends two signed copies of the MOU (or one digitally signed copy by fax or email) to the PC. Once reviewed and accepted by GML staff it is forwarded to NOAA administration for counter signature with one copy returned to the customer.
4. The PC prepares a work plan. The form of the work plan may vary, but should include a statement of work, calibrations required, ID numbers, and a target completion date. The work plan can be in electronic form created using custom software. Official approval from higher levels of management is not required to initiate a work plan.
5. The PC is the primary contact for the customer while the work plan is in place.
6. The PC implements the work plan and communicates requirements to a deputy PC and/or analysts as necessary. This can be done through direct contact, email, or software designed for this purpose.
7. When the work plan is complete, the PC or deputy PC queries results from a database. It is the responsibility of the analyst to ensure that data in the database are suitable for release to the customer.
8. The PC or deputy PC prepares an analysis certificate.
9. Certificates and calibrated items (gas cylinders) are sent to the customer.

7.1.2 GML offers only specific measurement services, available from a list, posted on the GML/CCL website or listed in an MOU template. Only services associated with GML's function as a CCL are accompanied by a certificate of analysis. If a material to be analyzed has not been prepared by GML, and presents analytical or commutability challenges, GML will, at its discretion, following communication with the customer, prepare an analysis report in lieu of a certificate.

7.1.3 GML does not offer "pass/fail" or "within tolerance/out of tolerance" services.

7.2 Selection, verification, and validation of methods

7.2.2 Selection and verification of methods

Methods described in Technical Procedures are known as GML methods. GML methods (or the results thereof) have been presented at WMO/GAW meetings and/or published in the peer-reviewed literature. Major changes in analytical methods, to the extent that the changes affect

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calibration results, are discussed within the WMO/GAW community. Any deviation from GML methods should be documented.

When standard methods, such as those developed by consensus standards development organizations, are available, GML will consider the use of standard methods. Use of standard methods may be discussed at WMO/GAW meetings or through consultation with WMO/GAW personnel.

Deviations from methods described in technical procedures should be discussed with the customer prior to accepting the calibration work order. If a need for deviation arises after the work order is accepted, the customer should be notified. Some reasons for deviating from GML methods might include: (a) the gas or sample container differs from what was specified in the agreement, or differs from what is used by other WMO/GAW laboratories; (b) the pressure is too low to apply GML methods, (c) the requested calibration is outside the range of the WMO/GAW scale, (d) unforeseen circumstances prevent the use of GML methods. Deviations from GML methods should be noted in analysis certificates. Any additional uncertainties associated with a deviation of the method should be communicated to the customer.

7.2.2 Validation of methods

GML critically evaluates all methods used for official measurements. GML methods are documented and evaluated through any of the following ways: (a) peer-review literature, (b) scientific meetings, including WMO/GAW meetings, (c) WMO/GAW reports, (d) NOAA technical reports. It is not necessary to demonstrate and document every aspect of method validation at every use of the method. The GML analyst may use documented evidence from prior applications of the method to demonstrate validity. For example, the working range of the method may have been demonstrated in a published paper. Methods that have yet to be published may be validated by comparison to existing methods, or by comparison of existing standards. Methods are validated over a specific mole fraction range corresponding to the WMO/GAW scale. Method validation may include:

- testing selectivity and specificity
- testing valid range
- evaluating sources of bias
- evaluating a response function (linear, polynomial, etc.)
- demonstrating reproducibility over a specified range or at a specified mole fraction
- routine monitoring of control standards
- comparing results to those achieved through other validated methods

7.3 Sampling

In general, GML does not calibrate sub-samples of a reference material in lieu of analyzing the reference material itself. In some cases, analysis of a sub-sample may be requested by the

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customer and these are handled on a case-by-case basis. This would normally be done for quality control purposes and would not be considered an official calibration.

7.4 Handling of test or calibration items

7.4.1 GML is committed to the safe and secure handling of calibration materials.

7.4.2 Gas cylinders are identified by stamped serial number. This number is used for all references to a particular calibration project, including data stored in the database. A “fill code” is used to designate different fillings of the same cylinder. A calibration project is tracked through different measurement stages through software designed for this purpose, and by attaching a paper work order to the cylinder. Each analyst initials the work order and records the date his/her calibration responsibilities have been completed. The PC verifies that the results are consistent with expectations.

7.4.3 The PC is responsible for working through all abnormalities that might occur during preparation and calibration stages.

7.4.4 Assessment of homogeneity: Since GML does not produce reference materials in batches, and each RM is individually analyzed, the only significant requirement to ensure homogeneity is that the gases are well-mixed prior to analysis (see the Technical Procedure for Reference Material).

7.4.5 Assessment of stability: Knowledge of reference material stability is important to GML and WMO/GAW. Multiple methods are used to assess stability (see Technical Procedures).

7.4.6 Characterization of reference materials: GML characterizes reference materials through quantitative value transfer (value assignment) from a suite of primary standards using a measurement procedure performed in our laboratory. Value assignment may involve multiple steps and is independent of the measurement procedure, within uncertainties specified on certificates.

7.4.7 It is GML policy to store cylinders and other materials for calibration in a secure environment. It is the responsibility of the TLs and analysts to ensure that gas use during the calibration process is not excessive. In most cases, a brass GCA-590 plug is used to ensure that cylinders are not “blown down” during transport. The PC should report any mishandling to the customer. Repairs (if warranted) are handled on a case-by-case basis.

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7.5 Technical records

Data corresponding to measurement results are stored electronically. Technical records pertaining to procedures, maintenance, and known problems are stored in an electronic log (ELOG). Each member of the CCL has access to the ELOG, and contributions are recorded with reference to username. Daily records, such as analysts notes, may also be recorded in log books associated with specific instruments or activities, and identified as such. While it is not necessary to duplicate all records in the ELOG, significant events should be recorded in the ELOG. Log books should include the name of the person entering information and date of entry. Electronic files are normally associated with a particular instrument and can be traced to personnel through logs.

7.6 Evaluation of measurement uncertainty

All analysis values reported on analysis certificates, or in association with official measurements, are accompanied by quantitative statements of uncertainty. Measurement results without uncertainties shall be explicitly labeled in the certificate as information values. Details of the measurement uncertainty assessment are contained in the TP-level documents, supplemental documents, or in published literature. Since GML methods are not updated frequently, measurement uncertainty is not evaluated for each individual measurement result individually as long as factors influencing uncertainty are under control. Instead, uncertainty budgets are evaluated for typical analytical conditions over a range of mole fractions.

7.7 Ensuring validity of results

7.7.1 GML uses several methods to ensure validity of results, which may include:

- analysis of control standards (also known as "target tanks" or "surveillance cylinders")
- retesting of items with previously assigned values
- intermediate checks on measuring equipment
- monitoring of metadata (engineering parameters)
- monitoring of instrument performance (e.g. repeatability)

Outliers should not be excluded solely on the basis of statistical evidence until they have been investigated (ISO 17034:2016, 7.13.4).

7.7.2 To the extent permitted by resources, GML will participate in comparisons with other WMO/GAW laboratories and National Metrology Institutes (NMIs). Special priority will be

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given to "key comparisons" conducted under the auspices of the Comité International des Poids et Mesures (CIPM).

7.8 Reporting results

Results are stored in a database and are reviewed using custom software. Certificates are generated by querying the database to minimize human error. Certificates contain the following information:

1. title of document
2. name and address of laboratory performing measurement
3. general description of the material
4. unique identification of report
5. unique identification of the item calibrated (gas cylinder ID) *
6. method used
7. results (including scale name or identifier)
8. uncertainty estimates
9. statement of traceability
10. hazardous information
11. name of person authorizing report

** Note: We prefer to identify results by cylinder number only. Customer names and contact information are not included on certificates. All information pertinent to the result, including instrument codes, can be accessed using the unique cylinder number and fill code.*

7.8.1 Amendments to certificates

Analysis results for reference materials are available on-line, referenced by cylinder serial number. Web-based access of results has been endorsed by WMO/GAW. In cases where technical issues or approved scale changes might necessitate data reprocessing, with a possible change in a result, customers will be instructed to check the web-based database for updates (amended certificates will not be issued). Scale updates are discussed at WMO/GAW meetings and announced to WMO/GAW participants via an email list server.

7.9 Complaints

GML seeks feedback from customers in various forms, including surveys, direct communication (email and phone), and during WMO/GAW meetings. All staff members are responsible for assessing the significance of complaints, with guidance from technical leads or project coordinators, to ensure that the appropriate levels of GML management are aware of the complaints and approve of the responses thereto. Resolution of complaints should be

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accomplished by the PC or TL and may involve higher levels of management when necessary. Complaints should be logged using the GML ELOG system and include:

- 1) the nature of the complaint, date received, name of person registering the complaint, GML recipient (if applicable), and initial response to the complainant
- 2) the final resolution of the complaint
- 3) a brief summary of all follow-up and the final communication with the complainant

7.10 Non-conforming work

Technical leads, analysts, and project coordinators share responsibilities for control of non-conforming work (i.e., calibration work that does not conform to GML policies and procedures, or is otherwise deemed to be sub-standard). This includes evaluation of the significance of the non-conforming work. If a non-conformity is identified, the nature of the non-conformity should be documented and brought to the attention of the technical lead. Analysts, project coordinators, and technical leads should communicate collectively and assess the significance of the non-conformity, and agree on a plan to address the issue. The scope of the plan will depend on the significance of the non-conformity.

If there is evidence, derived from any source, including customer feedback, that results of a calibration are unreliable or if the technical requirements specified in the MOU are not met, the PC should be notified and discussion with the customer should ensue.

When non-conforming or substandard work is identified, the particulars should be recorded in the ELOG, and summarized in semi-annual status updates. At a minimum, the following should be documented:

- a) significance of the non-conforming work
- b) when the nonconformity was discovered and the impact on measurement services
- c) what was done to determine root cause
- d) correction efforts required or taken
- e) customer notification, if deemed necessary
- f) delay or work stoppage, if deemed necessary

Analysts have the authority to stop calibration activities in the event that non-conforming or substandard work is identified or suspected. If the work stoppage leads to a significant delay, as determined by the analyst, the technical lead should be notified. The group chief should also be notified if the situation results in severe disruption of calibration activities.

If it is known in advance that an item for calibration cannot be calibrated under normal conditions, the customer should be contacted to discuss the issue. The PC, in consultation with TPs or analysts, will then determine an alternate course of action and proceed with customer approval. This may lead to issuance of an analysis report in lieu of a certificate (see section 7.1.2).

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GML is not responsible for non-conformities beyond GML control. Possible reasons for non-conformance beyond GML control include but are not limited to: a) inability to analyze a customer-supplied gas cylinder due to issues with gas connections, valves, etc. (b) erratic, unusually variable, or unstable behavior of trace gases in customer-supplied cylinders, and (c) inability to meet technical specifications due to unforeseen circumstances. With respect to reference materials, an inability to match all target mole fractions requested in the MOU is not considered non-conforming work. It is left to the PC to interact with the customer to reach agreement on targeted and resultant mole fractions.

If it is determined that non-conforming work is likely to reoccur, corrective and preventive action should be taken. The decision to implement minor corrective action may reside with analysts and technical leads. Major corrective actions, such as those requiring major purchases or procedure changes should involve the technical lead and group chief.

7.11 Control of data and information management

The laboratory information management system(s) used for the collection, processing, recording, reporting, storage or retrieval of data shall be validated for functionality, including the proper functioning of interfaces within the laboratory information management system(s) by the laboratory before introduction. Software changes should be documented and validated before implementation. Data transfer processes are checked in an appropriate and systematic manner (see Technical Procedures).

The laboratory information management system is accessed by username and password. The system is backed up regularly. Some areas of the information management system are restricted to particular users to prevent unauthorized data entry. In general, GML information management software is managed in-house, rather than managed off-site. Personnel are trained in-house on the use of in-house software.

8.0 Management system requirements

8.1 Options - GML elects to follow Option A of ISO 17025 - 2015. GML does not seek registration to ISO 9001.

8.2 Management system documentation

The official version of the GML quality manual and related sub-level documents are maintained on the GML server [//vnx4/CCL], readily available to all GML staff.

8.3 Control of management system documents

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The official version of the quality manual main document, GML-QM, and sub-level documents are read-only documents. Uncontrolled (read/print-only) copies are available external to GML on the GML website [<http://www.esrl.noaa.gov/GML/ccl/>]. GML servers have appropriate security and backup systems in place.

8.4 Control of records

After a revision of GML-QM is approved as the official version, GML personnel associated with the CCL are notified that an updated version of GML-QM is available on the GML server. Document changes will be recorded using the MS Word tool "Track Changes". In the event that substantial changes are needed, a statement of substantial changes should be included. A copy of the official version as well as obsolete versions (clearly marked as obsolete) of GML-QM documents shall be maintained on a separate backup system.

Critical records of calibration and traceability are stored in summary form on GML computer systems. Third-party calibration certificates In some cases, critical information related to calibration or traceability will be posted on or near instrumentation.

Records of customer interaction are maintained using commercial software designed for this purpose (GML ticket management system, or open-source ticket request system "OTRS"). Written interaction with customers (primarily by email) is logged and archived in OTRS. Records of phone conversations and emails outside the OTRS system are entered, in summary form, in OTRS (typically by the PC).

Technical records

Data records pertaining to analytical results may include data stored during analysis, processing, and testing. Data may be generated and stored in digital form using commercial or custom software. Critical electronic records are regularly backed up to secondary storage. The analysts and TLs determine which electronic records are critical to calibration actions. Paper records (notebooks, log sheets, etc.), if any, are kept in notebooks or binders. The identity of the analyst performing a procedure, measurement, or test may be kept in electronic or paper form. Maintenance records for instruments and associated devices are stored in the ELOG. The ELOG is also used to record significant events related to the performance of analytical instruments.

Analysis Results

Analysis results are stored in a database. Analysis results are made available on the GML website in anonymous form, searchable by cylinder number.

8.5 Actions to address risks and opportunities

GML should consider risks and opportunities as they relate to the function of the CCL and support of WMO/GAW, including opportunities to prevent, or reduce, undesired impacts and potential failures. Actions taken to address risk and opportunities should be proportional to the

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potential impact on laboratory results. Customer feedback will be an important input. Information gathered at WMO/GAW technical meetings is also important with respect to addressing risk and opportunity. GML recognizes that the hierarchical nature of calibration scale development and maintenance inherently reduces the risk of catastrophic failure (e.g. loss of a primary standard may lead to slightly higher uncertainties, but does not invalidate the scale).

8.6 Improvement

It is GML policy that all staff involved in calibration work use their analytical training and experience to identify needed improvements and/or potential sources of non-conformities (technical or managerial). Suggestions for actions can be discussed during annual status review meetings, or brought to the attention of technical leads or group chiefs. The software system used to log customer interactions can be used to analyze the effectiveness of the quality management system.

8.7 Corrective actions

If non-conforming work is identified, the PC shall work with TLs or analysts to identify the root cause, and if warranted, notify the customer. The PC, analyst or TL (as specified in lower level documents) shall have authority to proceed with the work after corrective action is taken. Repeated occurrence of non-conformities should be addressed at the TL or group chief level. An internal audit may be initiated to address root cause.

If a non-conformity, for which GML is responsible, is not discovered until after the customer receives the standard and the non-conformity cannot be addressed to the customer's satisfaction in any other way, GML will reanalyze the standard or attempt to provide a replacement standard at no cost to the customer.

Corrective actions will be documented in the ELOG system and summarized in semi-annual reports. Corrective action could lead to changes in the Quality Manual.

Non-conformities that have no significant impact on the quality of work will be logged and addressed when feasible, but may not require work stoppage or corrective action. TLs and PCs will evaluate the significance of minor non-conformities and plan appropriate action.

8.8 Internal audits

GML will perform internal audits at least every other year. Audits shall include QM documentation, traceability, actions and action logs, and a random check of certificates. Semi-annual status reports (see 8.9) serve as additional information pertinent to audits.

8.9 Management reviews

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GML will prepare semi-annual CCL status reports and meet annually to review and discuss activities related to conformance with ISO 17025:2017 and ISO/IEC 17034:2016. Semi-annual reporting and annual CCL meetings alleviate the need for yearly management reviews. Suitability of policies and QM documentation can be addressed during annual CCL meetings or as needed.

GML will perform management reviews at least every other year. The review shall take account of suitability of policies and procedures, results from audits, customer feedback, changes in volume and type of work, corrective and preventive actions, complaints, feedback from staff, feedback received at GGMT meetings, resources, and training.

Additional sources of feedback related to the management of the CCL may include:

- a) GML science reviews, conducted every 4-5 years.
- b) peer review, conducted every 5 years
- c) WMO/IAEA Carbon Dioxide, Greenhouse Gas and Related Measurement Techniques (abbreviated as GGMT) meetings (held approximately every 2 years).
- d) AGAGE (Advanced Global Atmospheric Gases Experiment) meetings, in which GML staff members often participate, and often focus on technical aspects of measurement.
- e) meetings of the Consultative Committee on Amount of Substance: Metrology in Chemistry-Gas Analysis Working Group (CCQM-GAWG).

9.0 Appendix

9.1 Abbreviations

| | |
|--------|---|
| AGAGE | Advanced Global Atmospheric Gases Experiment |
| CCL | Central Calibration Laboratory (a defined role in WMO/GAW network) |
| CCQM | Consultative Committee on Amount of Substance: Metrology in Chemistry |
| CGA | Compressed Gas Association |
| DOT | Department of Transportation (USA) |
| ESRL | Earth System Research Laboratory |
| GAWG | Gas Analysis Working Group |
| GGMT | Greenhouse Gases and related tracer Measurement Techniques, formerly referred to as Meeting of Experts on CO ₂ and related Tracer Measurement Techniques |
| GML | Global Monitoring Laboratory |
| GSA | General Services Administration |
| ISO | International Organization for Standardization |
| MOU | Memorandum of Understanding |
| NESDIS | National Environmental Satellite, Data, and Information Service |
| NMFS | National Marine Fisheries Service |

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| NMI | National Metrology Institute |
| NWS | National Weather Service |
| NOS | National Ocean Service |
| OAR | Oceanic and Atmospheric Research |
| OMAO | Office of Marine Aviation Operations |
| PC | Project Coordinator |
| QM | Quality Manual |
| SFF | Sales Fixed Fee |
| TL | Technical Lead |
| WMO | World Meteorological Organization |

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