# WDCGG Contributor Manual

# Chapter 1 2018 WDCGG website update

## 1. 1 Objectives of the 2018 WDCGG website update

Since the establishment of the World Data Centre for Greenhouse Gases (WDCGG) in 1990, requests from data contributors and users have included:

- a. Notifications regarding data usage (e.g., user names/affiliations, purposes of data usage) to contributors
- b. Unification of archive data file formats in various categories to a single format for users' simplified computer processing.

Certain types of observation data do not correspond fully with the format of metadata in the WDCGG database due to inappropriate metadata updates. As this causes issues with data utilization and hinders WDCGG staff efforts to develop database management and data services, WDCGG has enhanced the database and strengthened links between observation data and metadata. In tandem with these improvements, WDCGG has also updated its official website and data submission procedures.

## 1.2 Data submission changes

In the previous WDCGG system, data were sent by email, metadata were updated via an online form by contributors, and there was no procedure for user identification. Now there is an online registration page for contributors and users.

Major changes regarding data submission on the WDCGG website:

- a. Contributors are strongly encouraged to submit both observation data and corresponding metadata online.
- b. Previously there was no particular metadata format. Now certain metadata elements (e.g., aims of observation) are submitted with ready-made descriptions.
- c. A single standard data file format for submission independent of observation platforms is defined to facilitate final data usage.

# Chapter 2 Before data submission

Before submitting data, contributors need to sign up for an account on the WDCGG website (<a href="https://gaw.kishou.go.jp/">https://gaw.kishou.go.jp/</a>). Accounts are assigned to organizations rather than to individuals.

Organizations new to WDCGG can register at <a href="https://gaw.kishou.go.jp/login/contributor">https://gaw.kishou.go.jp/login/contributor</a>.

To submit new data after logging in, click "New Data Registration" and register the information to be provided.

# Chapter 3 Data submission

Contributors log in, click "Data/Metadata Submission" and follow five simple steps to submit data as outlined below.

# 3.1 Step 1. Select Data Catalogue

Check the relevant gas species for each station from which data is to be submitted. At least one box must be checked.

If the data to be submitted are not listed, click "New Data Registration" on the post-log-in page.

# 3.2 Step 2. Input Metadata/Edit Metadata

To input or edit metadata, select the item, click "Edit" and fill out the form on each page. "Organization," "Contact," "Aim of Observation," "Data Time Zone" and "Unit" are required fields. Once metadata input or editing is complete, click "Next" at the bottom of the page.

# 3.3 Step 3. Check Metadata

Check the updated metadata carefully. To edit, click "Back" at the bottom of the page to return to Step 2; otherwise, click "Next."

# 3.4 Step 4. Check Station

Check the station information from the GAW Station Information System (GAWSIS). Check and edit the mobile station information stored in the WDCGG database as needed. The station/mobile information here is shown in the header part of the WDCGG data file. Latitude, longitude and altitude values differing from GAWSIS values should be included in the data part of the file. Then, click "Next."

Be sure to check the station information. WDCGG just obtains station information from the GAWSIS. Please update the station information on the GAWSIS website as needed.

## 3.5 Step 5. Upload Datafile

Up to five files (< 10 MB each) can be selected and uploaded by clicking "Submit." Submission of single compressed files is preferred. Meteorological data can also be uploaded.

Limit: 5 files (< 10 MB each)

Permitted file types: csv, txt, dat, xls, xlsx, prn, zip, tar.

To avoid inappropriate updates to data and metadata, contributors should submit the whole available body of observation data and corresponding metadata each time to ensure that WDCGG information matches the latest version of the data which contributors have.

Contributors are encouraged to submit monthly data as well as event/hourly/daily data. As WDCGG uses monthly data in analysis for the WMO Greenhouse Gas Bulletin and the WMO WDCGG Data Summary, monthly data may be derived from hourly or daily data submitted with no monthly data. For more information on the calculation procedure, see

https://gaw.kishou.go.jp/static/documents/wdcgg\_data\_format\_table.pdf.

Regarding meteorological data, only event and hourly meteorological data are collected. Some meteorological data published on the previous WDCGG website could not be converted to the new meteorological format. Contributors are asked to resubmit these data in the new format.

Contributors should input the URL to have WDCGG retrieve files from their FTP servers.

Descriptions relating to meteorological data (e.g., anemometer heights, wind speed sampling methods when it is not average wind speed for the previous 10 minutes) can be noted at 5.2 on the form.

Enter the name and email address and click "Submit."

Follow the online instructions for "Data/Metadata Submission." WDCGG will contact contributors at the email address provided once data processing is complete.

# Chapter 4 Metadata Submission

Observation data and metadata should be updated in a timely manner to ensure that WDCGG data matches the latest version of submitters' data. Contributors are asked to submit details of stations, observations and other related information as metadata. As these data are indispensable for effective usage, descriptions should be as outlined on the WDCGG website. Required fields are marked with a red asterisk. Changes in metadata such as calibration scales and observation instruments can be specified (via submission) for the corresponding period. To delete metadata, leave the field blank and proceed to the next step.

## 4.1 Organization\*

This is information for the organization submitting the data to WDCGG and primary contact from WDCGG or users. The organization's name, acronym and country/territory are required. Fill out the Organization Acronym field using upper and/or lower case letters, like "WDCGG" or "Empa," in 2 to 16 characters. The table on the page shows contributor information as registered on the WDCGG database. Information should be double-checked and modified as necessary before submission.

### 4.2 Collaborator(s)

Institutes or organizations collaborating with the contributor. The organization's name, acronym and country/territory are required. The organization acronym should be entered using upper and/or lower case (e.g., WDCGG), and should be between 2 and 16 characters.

Up to three collaborators can be chosen from the drop-down list at one step.

Individual collaborators who should not receive inquiries, requests or other forms of contact regarding submitted data can be specified on the second page. Any individuals specified must be members of the collaborating organization indicated on the first page, but specification of individuals is optional.

### 4.3 Contact\*

The contact is the person responsible for handling inquiries, requests and other forms of consultation regarding submitted data. At least one person must be registered, and multiple contacts are preferable. WDCGG and data users can email the contact directly.

Contacts can be chosen from the drop-down list. If no list entries are applicable, add contact details as necessary (name, organization, role, country/territory and so on).

### 4.4 Aim of Observation\*

Select an "Aim of Observation" option such as "Background observation." If none of the options applies, specify the aim in the box that appears after the "Other" option is selected. Entering "Unknown" is discouraged.

### 4.5 Data Time Zone\*

Time zones are defined by the time offset (i.e., the difference between local time and UTC (local time – UTC)) from Coordinated Universal Time (UTC). Select the time zone for the timestamp of the observation data. If none of these applies, specify the relevant information after selecting the "Other" option. Entering "Unknown" is discouraged.

### 4.6 Unit\*

Select the unit used for the observation data. If none of these applies, specify the relevant information after selecting the "Other" option. Entering "Unknown" is discouraged.

### 4.7 Calibration Scale

The calibration scale used for observation data and the period of the scale's usage should be indicated here. If the period is equal to the entire period of the observation, input the date and time as follows:

Start date and time: 9999-12-31, T00:00:00

End date and time: 9999-12-31, T23:59:59

Use the time zone specified in 4.5. Indications of "unknown" are discouraged for CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O in particular.

## 4.8 Instrument(s)

Indicate the characteristics of the measurement instrument(s). The applicable data period, manufacturer, product name, model number and measurement method should be specified. If the metadata are equal to the entire period of observation, input the date and time as follows:

Start date and time: 9999-12-31, T00:00:00

End date and time: 9999-12-31, T23:59:59

Use the time zone specified in 4.5.

If event data measured using multiple instruments for a specific period can be treated as a single data series, indicate the correspondence between instruments and each data line directly in the instrument and measurement method columns for the data submitted.

# 4.9 Intake Height above ground level

The height (depth) of air (seawater) sampling above the ground (below sea level) in meters: positive for height and negative for depth, except for mobiles (3D) whose altitudes are included in the observation data. Metadata being equal over the entire period of the observation, input the date and time as follows:

Start date and time: 9999-12-31, T00:00:00

End date and time: 9999-12-31, T23:59:59

Use the time zone specified in 4.5. For mobile platforms, leave the field blank or input "NA."

The height (depth) indicated here must be consistent with the intake height columns for the submitted data.

(height in submitted data # height (depth) in metadata

Note that Altitude = Elevation + Intake height. See also 5.3 Data record format.)

Alternatively, enter "-999.999" in the intake height columns for the submitted data to have WDCGG complete each data line based on the height (depth) indicated here.

# 4.10 Sampling Frequency

Select the periodicity of raw data sampling for the current observation. If none of these applies, specify the relevant information after selecting the "Other" option. Entering "Unknown" is discouraged.

## 4.11 Measurement Calibration

Contributors should indicate the details of measurement calibration. Calibration for determining mole fractions is described here along with procedures for analysis such as the order of introduction (sequence) for sample and standard gases (or zero gases) to the instrument, the relevant time period and the number of calibration points.

### Example 1 (CO<sub>2</sub>)

The quadratic fitting curve is determined every two hours based on a set of five working standard gases consisting of CO<sub>2</sub>-in-natural-air mixtures with different concentrations. The mole fraction is determined from this fitting curve.

### Example 2 (CH<sub>4</sub>)

Ambient and standard air samples are injected into a gas chromatograph (GC) with a sampling valve. Methane (CH<sub>4</sub>) is separated from other sample constituents using packed columns and detected using flame ionization (FID). This process is highly automated for field and laboratory operations. The instrument response for the sample must be compared to a standard with known CH<sub>4</sub> content.

## 4.12 Data Processing

Details of instrumental data processing are described here. Criteria used in selection for data processing should also be described.

#### Example

Raw data from the instrument are collected via the data acquisition system and stored as raw data for each 30-second period. CO<sub>2</sub> observations are checked on site by an operator every day.

## 4.13 Processing for averaging

Details of processes on hourly, daily, monthly data or data selections regarding quality are to be provided here. Individual specifications on how hourly, daily and monthly averages are calculated can be given by selecting "Hourly", "Daily" or "Monthly" first. Be sure to select the appropriate radio button.

#### Example

Processing of hourly data: Data are taken from the arithmetic mean of observations covering a one-hour period after rejection of irregular data and obvious errors.

# 4.14 Original Data Quality Flags

Indicate the criteria for data flagging. If data are already marked with WDCGG data quality flags in the next item description, original data quality flags may not be necessary depending on metadata for the next Data Quality Flag (Valid/Invalid) item.

### Example 1:

Flag: Data Category

- 0: Background data
- 1: Data possibly affected by pollution (wind direction is W SW)
- 2: Insufficient number of averaging data
- 3: Invalid data

#### Example 2

NOAA ESRL uses a 3-column quality control flag where each column is defined as follows:

column 1 Rejection flag. An alphanumeric other than a period (.) in the FIRST column indicates a sample with obvious problems during collection or analysis. This measurement should not be interpreted.

column 2 Selection flag. An alphanumeric other than a period (.) in the SECOND column indicates a sample that is likely valid but does not meet selection criteria determined by the goals of a particular investigation.

column 3 Information flag. An alphanumeric other than a period (.) in the THIRD column provides additional information about the collection or analysis of the sample.

WARNING: A "P" in the 3rd column of the QC flag indicates the measurement result is preliminary and has not yet been carefully examined by the PI. The "P" flag is removed once the quality of the measurement has been assessed.

## 4.15 Data Quality Flag (Valid/Invalid)

WDCGG has introduced its own preliminary data flagging scheme to make data files machine-readable. There are three basic types: "1 valid as background", "2 valid", and "3 invalid". Indication should be provided on how flags relate to these three types.

This description helps to clarify the relationship between contributors' original data quality flags and WDCGG data quality flags, and eliminates the need to input "QCflag" item values in data records as described in 5.3.

## 4.16 Reference(s)

References to the observation (such as the instruments, data processing, and calibration) in the literature or URLs should be described here.

Data citations can also be provided here.

### 4.17 Observation Status

Select the most appropriate current description from "Operational/Reporting," "Temporarily suspended" and "Terminated." Updates should be provided as appropriate.

The status will automatically change to "Temporarily suspended" 27 months after the last submission.

# 4.18 Description

Any other information on observations or data can be provided here.

Available information on long/short-term analytical stability and calibration/scale transfer uncertainty of data can be specified.

### 4.19 DOI

Select "Request for WDCGG DOI issuance," "Original DOI already present" or "Undecided." Contributors selecting "Original DOI already present" should provide the DOI.

# Chapter 5 Data File Names and Record Formats

#### 5.1 Data file names

WDCGG employs the following naming convention:

{ WDCGGParameterCode }\_{ SiteGawId }\_{ Platform }-{ SamplingType }\_{ Organization Code }\_{ DataType }.txt

The file name for relevant meteorological data should be as follows:

{ WDCGGParameterCode }\_{ SiteGawId }\_{ Platform }-{ SamplingType }\_{ Organization Code }\_{ DataType }\_met.txt

File names consists of WDCGGParameterCode, SiteGawId, Platform, Sampling\_Type, OrganizationCode and DataType. These must be delimited with underscores ("\_") and dashes ("-").

#### Example

co2\_mnm\_surface-insitu\_1\_monthly.txt

This expresses:

 $co2\ (WDCGGParameterCode)\_mnm(SiteGawId)\_surface(Platform)-insitu(Sampling\ Type)\_1(Organization\ Code)\_monthly(DataType).txt$ 

#### (1) WDCGGParameterCode

This code identifies an observing gas species.

For meteorological data, the relevant gas parameter code (rather than "MET") should be set.

Details: https://gaw.kishou.go.jp/documents/db list/gas species

#### (2) SiteGawId

Three-letter codes in lower case are used to identify stations. For GAW stations, GAWSIS station IDs are employed.

Details: https://gaw.kishou.go.jp/documents/db\_list/station

#### (3) Platform

This code identifies a platform at which observation is performed.

Details: https://gaw.kishou.go.jp/documents/db list/platform

#### (4) SamplingType

This code identifies a sampling type.

Details: https://gaw.kishou.go.jp/documents/db\_list/sampling\_type

#### (5) OrganizationCode

This number is used to identify a contributor's affiliation.

Details: https://gaw.kishou.go.jp/documents/db list/organization

#### (6) DataType

This field indicates the temporal resolution for each data record.

Details: https://gaw.kishou.go.jp/documents/db list/data type

### 5.2 Header records

Header records are created automatically from metadata registered by data contributors. Lengths are variable and defined at the top of the record. For more information, see

https://gaw.kishou.go.jp/static/documents/wdcgg\_data\_format\_table.pdf

https://gaw.kishou.go.jp/static/documents/wdcgg\_meteorological\_data\_format\_table.pdf

### 5.3 Data record format

### (1) gas data

Data records in the new WDCGG file format are as follows ("+" represents a space): [Site\_gaw\_id]+[Year]+[Month]+[Day]+[Hour]+[Minute]+[Second]+[Year]+[Month]+[Day]+[Hour]+[Minute]+[Second]+[Value]+[Value]+[Value]+[Nvalue]+[Latitude]+[Longitude]+[Altitude]+[Elevation]+[Intake\_height]+[Flask\_no]+[ORG\_QCflag]+[QC flag](+ [Instrument] + [Measurement\_method] + [Scale]).

### Example:

Composition items are as per the table below.

Table 1. Data record elements

Item	Number of digits	"No Data" expression	Content	Detail	
Site_gaw_id	3	-	Site code	3-letter site identification code as defined by GAWSIS for stationary platforms	
Year	4	-999	Start year	Initial calendar year of observation	
Month	2	-9	Start month	Initial calendar month of observation	
Day	2	-9	Start day	Initial day of observation	
Hour	2	-9	Start hour	Initial hour of observation	
Minute	2	-9	Start minute	Initial minute of observation	
Second	2	-9	Start second	Initial second of observation	
Year	4	-999	End year	Final calendar year of observation	
Month	2	-9	End month	Final calendar month of observation	
Day	2	-9	End day	Final day of observation	
Hour	2	-9	End hour	Final hour of observation	
Minute	2	-9	End minute	Final minute of observation	
Second	2	-9	End second	Final second of observation	
Value	Variable	-999.999	Observation value	Reported mole fraction, isotope ratio or radioactivity. Units depend on trace gas species.	
Value_unc	Variable	-999.999	Uncertainty based on standard deviation	Standard deviation of the reported mean value when Nvalue is greater than 1. Units depend on trace gas species.	
Nvalue	Variable	-9	Number of measurements	Number of individual measurements used to compute reported values	
Latitude	Variable	-999.999999999	Latitude	Latitude of sampling location in decimal degrees (north: +; south: -)	
Longitude	Variable	-999.99999999	Longitude	Longitude of sampling location in decimal degrees (east: +; west: -)	
Altitude	Variable	-999.999	Elevation + intake height	Altitude (elevation + intake height) of air sample collection. Units are meters above sea level (masl).	
Elevation	Variable	-999.999	Station height	Station height (m) above sea level	
Intake_height	Variable	-999.999	Sampling height	Sampling height (depth) of air (seawater) above ground (below sea level) (height: +; depth: –) (m)	
Flask_no	Variable	-999.999	Flask identifier	Identification code (or number) of flask used for observation	
ORG_QCflag	Variable	-999.999	Original data quality control flag	Details of original data quality control flags should be specified by contributors in metadata.	
QCflag	Variable (1 or 2)	-9	WDCGG data flag	1 Valid (background) data considered "background" 2 Valid data considered valid other than "background," or all valid data without categorization 3 Invalid data considered unfit for use (questionable/erroneous/absent data) Details of correspondence between original data quality control flags and WDCGG data flags should be specified by contributors in metadata.	

Instrument (Optional item)	Variable (1 or 2)	-9	Instrument number	Instrument sequence number from oldest to newest	
Measurement_method	Variable (1 or 2)	-9	Measurement method	Measurement method employed.	
(Optional item)			code		
Scale (Optional item)	Variable (1 to 4)	-9	Scale code	Employed scale in observation	

### (2) meteorological data

Meteorological data records in the new WDCGG file format are as follows (where "+"represents a space):

[Site\_gaw\_id]+[Year]+[Month]+[Day]+[Hour]+[Minute]+[Second]+[Wind\_direction]+[Wind\_speed]+ [Relative\_humidity]+[Precipitation\_amount]+[Air\_pressure]+[Air\_temperature]+[Dew\_point\_temperature]+[Sea\_water\_temperature]+[Sea\_surface\_water\_Temperature]+[Sea\_water\_salinity]+[Latitude]+[Longitude]+[Altitude]+[Elevation].

Table 2. Data record elements

Item name	Number of digits	"No Data" expression	Content	Explanation of the item
Site_gaw_id	3	-	Site code	3-letter site identification code as defined by GAWSIS for stationary platforms
Year	4	-999	Year	Calendar year of observation
Month	2	-9	Month	Calendar month of observation
Day	2	-9	Day	Day of observation
Hour	2	-9	Hour	Hour of observation
Minute	2	-9	Minute	Minute of observation
Second	2	-9	Second	Second of observation
Wind_direction	Variable	-99.9	Wind direction (degree)	Angle (in degrees) between true north and wind direction, and clockwise increase
Wind_speed	Variable	-99.9	Average wind speed (m/s)	Average wind speed for the previous 10 minutes. See note *1.
Relative_humidity	Variable	-99.9	Relative humidity (%)	
Precipitation_amount	Variable	-99.9	Precipitation amount (mm)	
Air_pressure	Variable	-999.9	Air pressure (hPa)	
Air_temperature	Variable	-99.9	Air temperature (degree Celsius)	
Dew_point_temperature	Variable	-99.9	Dew point temperature (degree Celsius)	
Sea_water_temperature	Variable	-99.9	Sea water temperature (degree Celsius)	Temperature at the observation point
Sea_surface_water_temperature	Variable	-99.9	Sea surface water temperature (degree Celsius)	,
Sea_water_salinity	Variable	-9999.9	Sea water salinity (permil)	Sea water salinity at the observation point as calculated using the Practical Salinity Scale 1978 (PSS-78; unit: permil)
Sea_surface_water_salinity	Variable	-9999.9	Sea surface water salinity (permil)	Sea surface water salinity as calculated using the Practical Salinity Scale 1978 (PSS-78; unit: permil)
Latitude	Variable	-999.99999999	Latitude	Latitude of sampling location in decimal degrees (north: +; south: -)
Longitude	Variable	-999.99999999	Longitude	Longitude of sampling location in decimal degrees (east:+; west: -)
Altitude	Variable	-999.999	Elevation + intake height	Altitude (elevation + intake height) of sample collection. Units are meters above sea level (masl). *2
Elevation	Variable	-999.999	Station height	Station height (m) above sea level

<sup>\*1</sup> Information on meteorological data (e.g., anemometer heights and wind speed sampling methods when it is not average wind speed for the previous 10 minutes) can be included in Step 5.2 during data submission.

<sup>\*2</sup> This column is used mainly for mobile platform data with varying intake heights (depths) for individual observations (e.g., 3000 for 3 km, -1000 for 1000 m depth). Enter "-999.999" for data that are

fixed for individual observations and varied for elements.

## [Revision history]

2018-08-31: Format Version. 1.0: Manual publication

 $2020 \hbox{-} 06 \hbox{-} 17 \\ \hbox{:} Format Version. \ 1.0 \hbox{:} Addition of information on meteorological data and other matters}$ 

2021-03-25: Format Version. 2.0: Addition of optional items on gas data format and DOI on metadata