DASIG Model Version 1
Comprehensive User's Guide

Version 1.0.2

Developed by the DASIG Team
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Foreword

DASIG Model Version 1 is a modular analytical suite developed to streamline the end-to-end processing of soil trace gas analytical data. DASIG Model is a user-friendly software application for calculating soil trace gases such as nitrous oxide (N_2O), methane (CH_4), and carbon dioxide (CO_2) from crop fields using the chamber method. The modular data processing software is written in Python and is packaged as a single installer program for Microsoft Windows, which contains all software requirements to run the model.

DASIG 1.0 consists of four sub-modules: GC-PREP, KASOKU, FLUX, and GWP. The GC-PREP submodule expedites the preparation and identification of gas samples for sequential run analysis using a model 2014 or 2030 Shimadzu gas chromatograph (GC) coupled with LabSolutions™ GC software version 5.111. The GC-PREP submodule focuses on gas sample identification, formatting, and creation of sequences of gas samples for GC analysis. The KASOKU submodule facilitates the integration and post-processing of GC data, creation and assessment of externally determined calibration curves, and computation of molar mass concentrations of gas using the Ideal Gas Law equation. The FLUX submodule calculates GHG fluxes from a time series of gas concentrations using either linear or non-linear time relationships. The GWP submodule converts GHG flux data into cumulative emissions throughout the crop cycle or crop season, expressed as CO_2-equivalents, using trapezoidal time integration.

Data validation of the DASIG model was conducted using six datasets from drill-seeded rice field studies in the USA and showed the GHG emission datasets computed by the DASIG model are significantly comparable to manually computed GHG emissions. Using the model, data processing time is shortened by > 1,000 times when compared to manual calculations.

All DASIG modules are managed from a common user interface, and the software package is distributed as a single installation program for Windows. Together, they enable scientists and technicians to move seamlessly from raw GC data to standardized CO_2-equivalent emission estimates.

This document serves as a user-friendly reference for both new and experienced users, emphasizing data integrity, repeatability, and analytical accuracy in GHG quantification workflows.

This automated tool is highly relevant in the determination of uncertainties for accurate inventory of GHG from crop production, validation of GHG models for agricultural crops, and as a platform to unify GHG datasets globally.

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Chapter 1: DASIG Model Installation

1. Overview

The DASIG model is distributed as a standalone Windows installer program, and does not require the installation of any other software. All dependencies are embedded within the installer program, which include both Python and *R* runtime environments, ensuring seamless installation and consistent performance across computer systems.

2. System Requirements

Category	Specification
Supported OS	Windows 10 / 11 (64 bit)
Distribution	Executable installer (.exe)
Processor	Intel / AMD Dual-Core or higher
Memory	4 GB minimum (8 GB recommended)
Storage	200 MB free disk space
Network	Optional (for installation)
Permissions	Write access to the selected output folder

3. DASIG Versions Compatibility

The DASIG software is updated frequently, as new features are added. At times, new features require that the format of input files are changed, making older files incompatible with newer versions. **Therefore, ensure the newest version is installed on all computers and the same version is used by all team members.** Please check the download websites listed in the next section to verify you have the newest version.

DASIG versions are numbered with 4 sequential digits (e.g. 1.0.1.0). The last digit is updated when minor improvements are made to the software, which do not involve changes in calculation results or incompatibility of inputs. Software changes that may affect computed fluxes or require adjustments of input files are indicated with an increased third digit, for example from 1.0.0.4 to 1.0.1.0. The following table shows the most important recent changes. All changes are listed in the installation Readme file, accessible from the Windows ***Start*** menu.

Version	**Important Changes**
1.0.2.0	Improvements to user interface and flux reporting.
1.0.1.1	Improvements to software installation.
1.0.1.0	Users may override the R2 value used to define GC calibration curves.
1.0.0.4	Improvements to user interface and output formatting.
1.0.0.0	Initial release.

4. Software Download

1. Download method for this installation

   Although DASIG is normally accessed and downloaded through the official GRA website after completing the registration form, this installation uses a direct download link provided by the project team. This link redirects users to the same official installer while allowing installation to proceed without completing the online registration process.

   For the best download experience, we recommend using Google Chrome or Microsoft Edge as the web browser.

   Depending on browser security settings, a warning may appear indicating that the file is not commonly downloaded or may pose a security risk. If this occurs, select “Keep” or “Keep anyway” to allow the installer file to be saved to your computer.

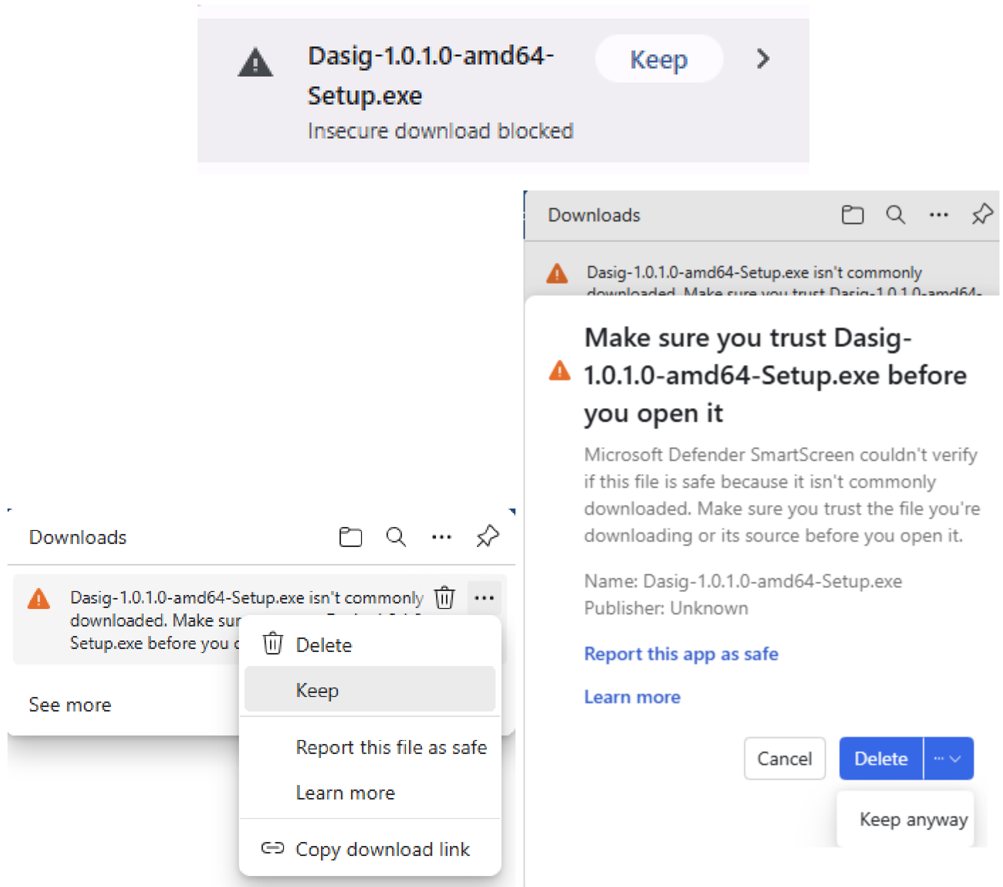


Figure 1.1. Examples of browser security warnings displayed during DASIG installer download in Google Chrome and Microsoft Edge.

DASIG installer files follow the naming convention Dasig-1.0.1.0-amd64-Setup.exe, where 1.0.1.0 denotes the DASIG software version. The suffix “amd64” indicates compatibility with 64-bit processor architectures, including both AMD and Intel systems.

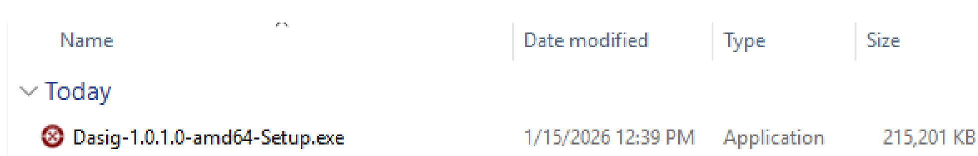


Figure 1.2. Example of the downloaded DASIG installer file (Dasig-1.0.1.0-amd64-Setup.exe) located in the system downloads folder.

When opening the downloaded setup application, a Windows security screen similar to the one shown below may appear. If this screen is displayed, select **“More info”**, then click **“Run anyway”** to proceed. Once confirmed, the installation process will begin.

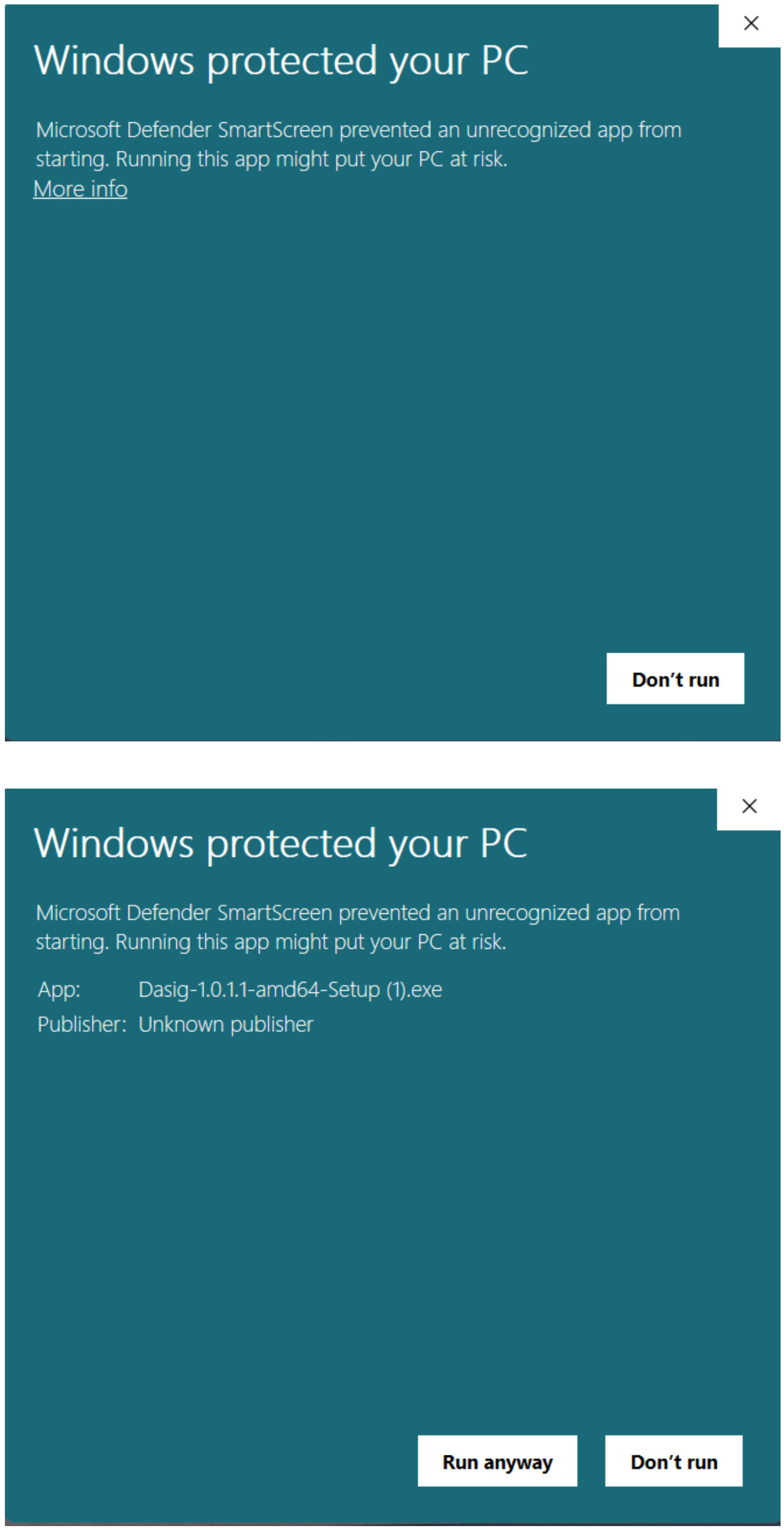


Figure 1.3. Windows Defender SmartScreen security prompt that may appear when opening the DASIG setup application.

2. Software installation

1. Installation mode
Locate the downloaded setup file on your computer and double-click to launch it. You will first be prompted to choose an installation model.

Select "Install for me only (recommended)" and click **Next** to proceed.

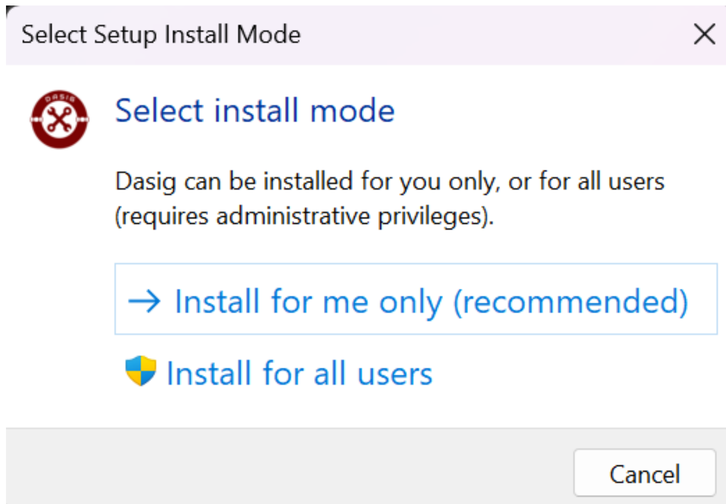


Figure 1.4. Installation-mode selection dialog shown during DASIG setup, indicating user-level and system-wide installation options.

DASIG can be installed for a single user, or for all users of a computer. The latter option requires administrative rights, while installing it for the currently logged in user does not. For most situations, installing DASIG for a single user is recommended.

2. Welcome and License Agreement

After launching the installer, the DASIG Setup Wizard opens and displays a welcome screen confirming the software version to be installed. It is recommended that all other applications be closed before proceeding. Click Next to continue with the installation.

The installer will then display the software license agreement. Review the terms carefully. To proceed with the installation, select “I accept the agreement” and click Next. Selecting “I do not accept the agreement” will cancel the installation process.

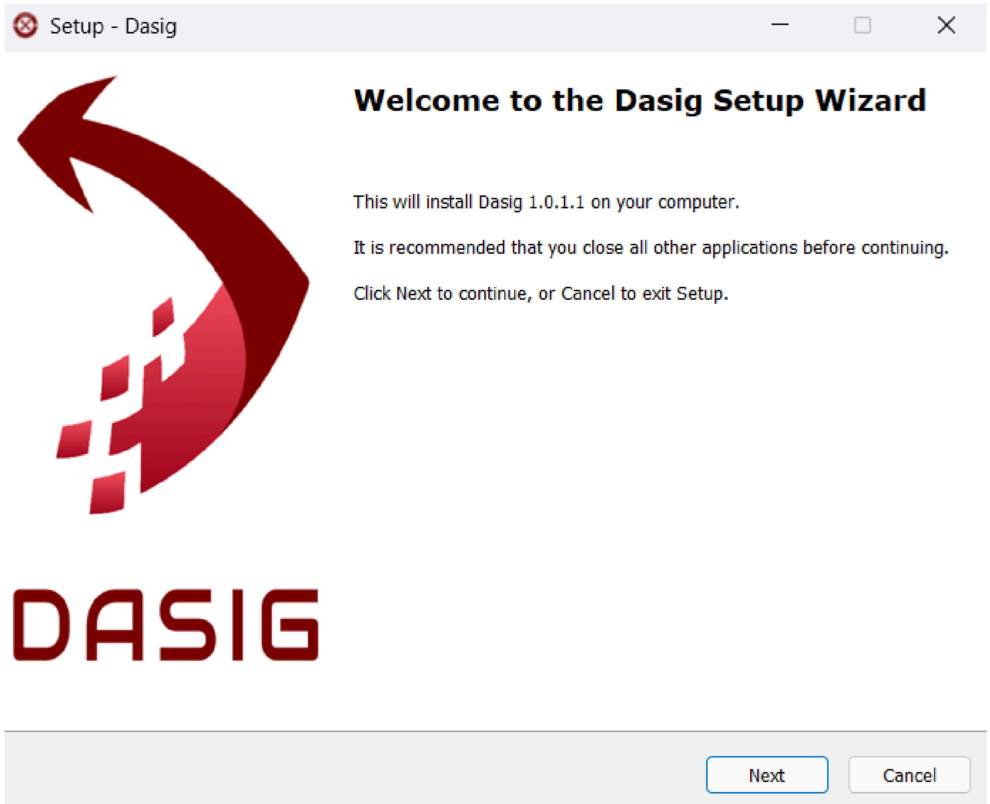


Figure 1.5. Welcome screen of the DASIG Setup Wizard displayed after launching the installer.

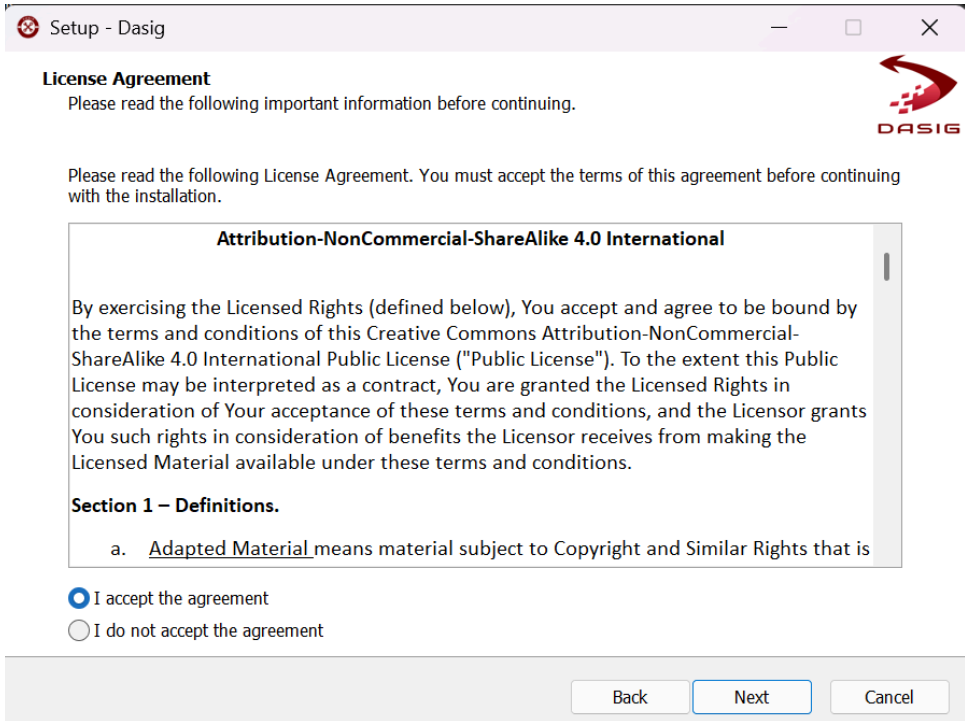


Figure 1.6. DASIG software license agreement screen. Users must accept the license terms to proceed with installation.

3. Installation Overview

The DASIG model requires the R statistical computing environment to operate. If R is not already installed on the user's computer, it will be installed automatically as part of the DASIG setup process. DASIG also installs the HMR R package, which is required for the computation of non-linear greenhouse-gas fluxes.

Both R and the required R packages are bundled with the DASIG installer. No additional downloads or user intervention are required. Users are prompted during installation to approve the installation of these dependencies.

Click **Next** to proceed with the installation.

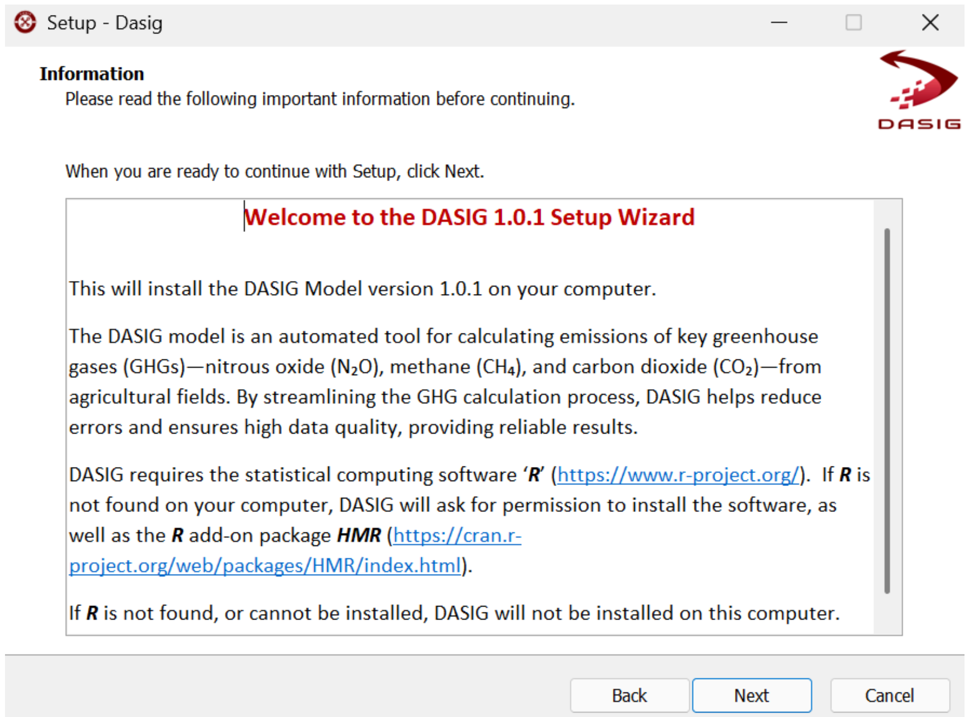


Figure 1.7. DASIG installation overview screen showing required dependencies, including R and the HMR package, prior to continuing with setup.

4. Optional: Create a Desktop Shortcut

   During installation, users may choose to create a Windows desktop shortcut for quick access to the DASIG application. If a desktop shortcut is desired, select the corresponding checkbox and click **Next** to continue. This step is optional and does not affect the core functionality of the software.

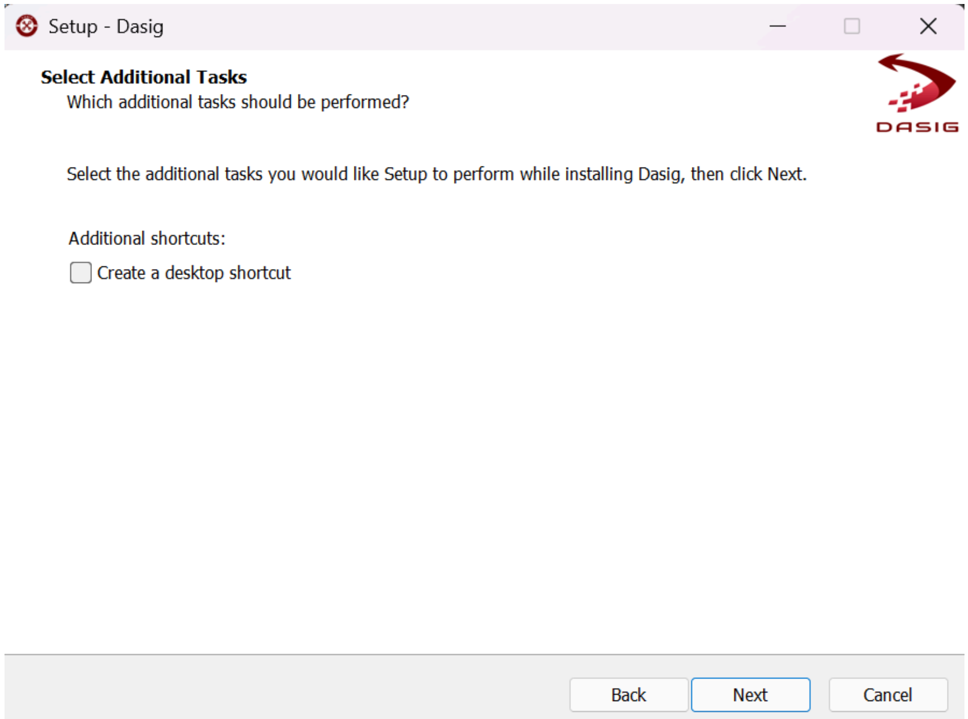


Figure 1.8. Optional selection screen for creating a Windows desktop shortcut during DASIG installation.

5. Installing DASIG and Dependencies
   The installer will begin copying files and configuring the application. If your PC does not already have the required version of R or the HMR package, a prompt will appear asking for permission to install these components. Select **Yes** to allow installation, then continue. The installation will then resume automatically.

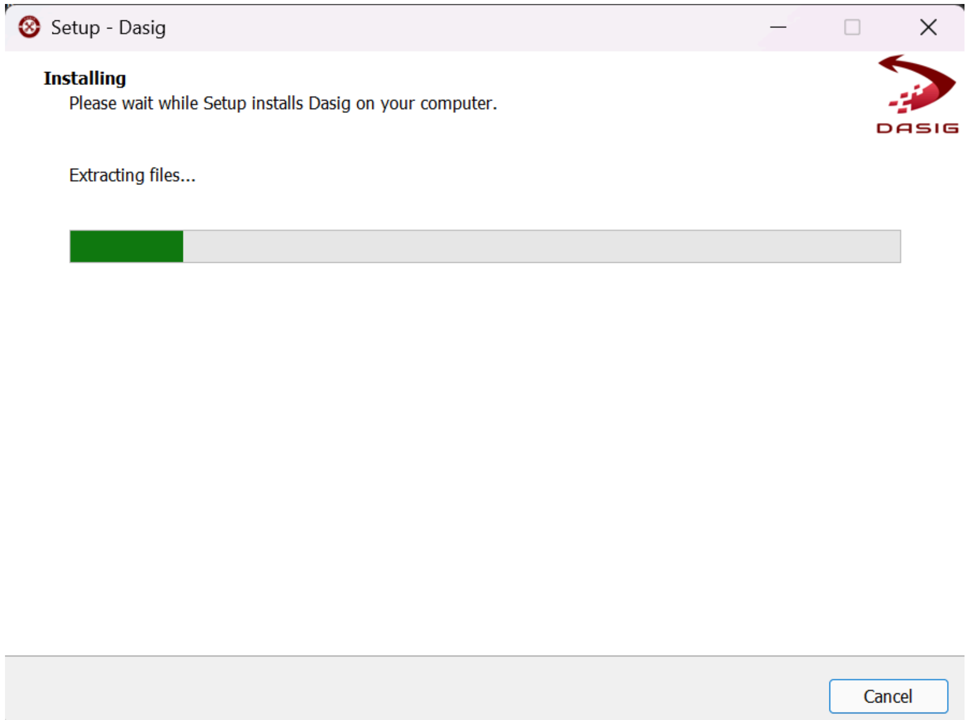


Figure 1.9. Initial DASIG installation progress window.

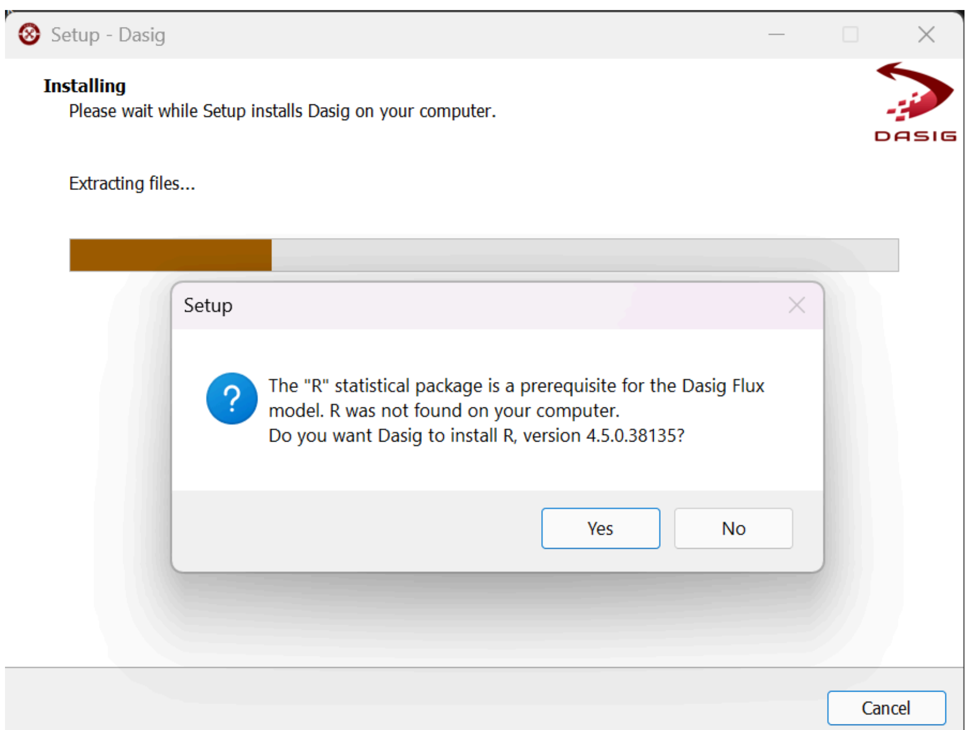


Figure 1.10. Dependency installation prompt for required R and HMR packages.

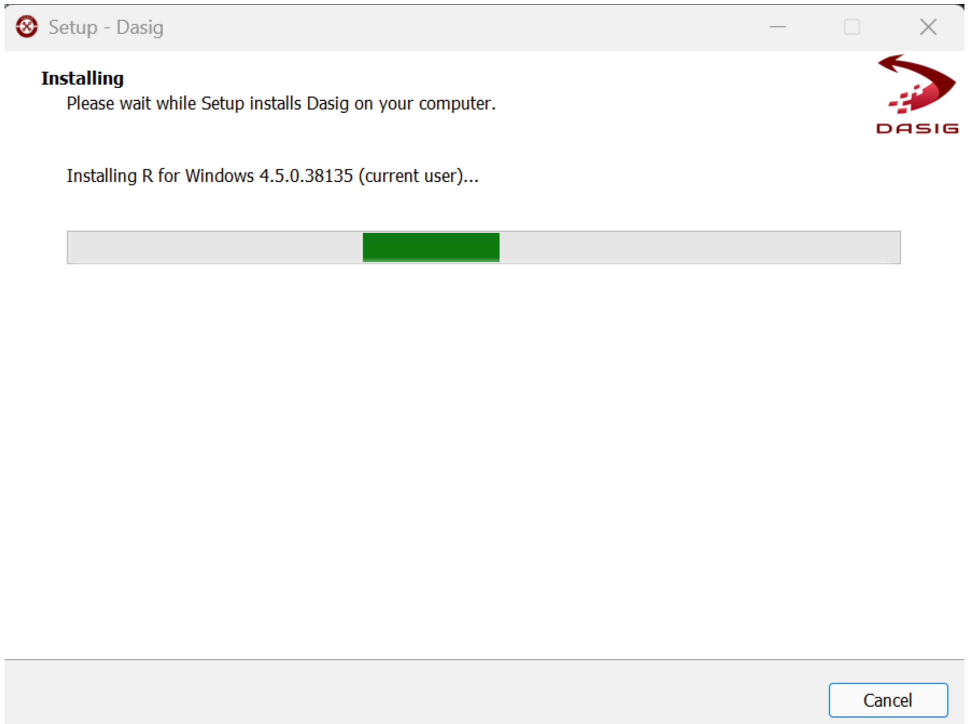


Figure 1.11. Completion of DASIG and dependency installation.

6. Completing the Installation
   Once the installation is finished, a confirmation screen will appear. Click **Next**, then Finish to exit the installer.

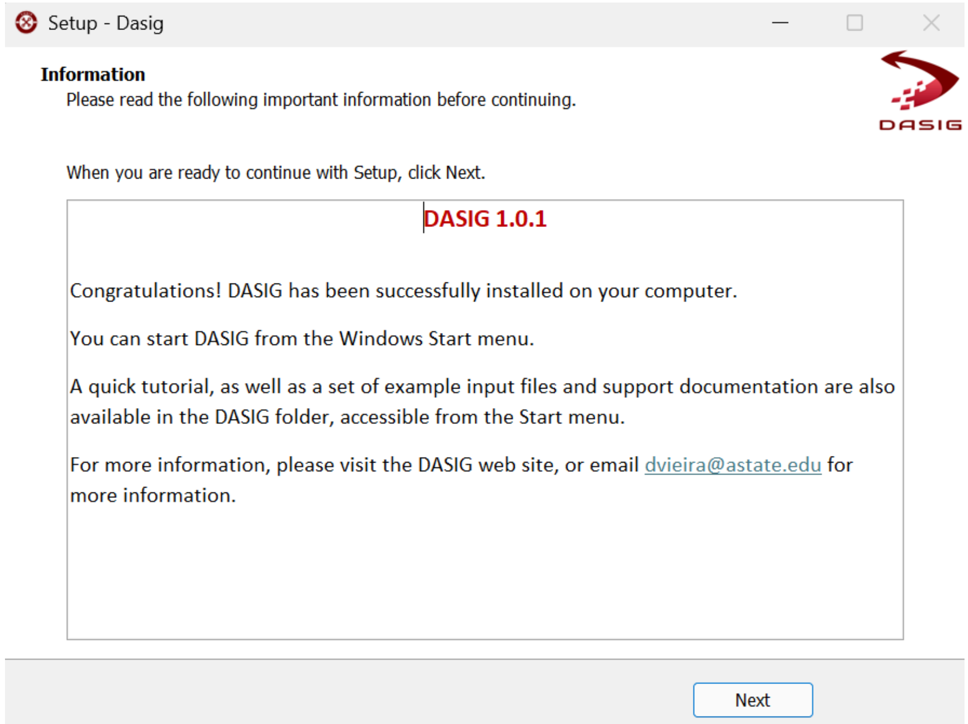


Figure 1.12. Completion of the DASIG Installation Process

7. Launching the DASIG Application

   If you chose to create a shortcut, you will now see the DASIG icon on your Windows desktop. Double-click the icon to launch the DASIG application and begin using the model.

   DASIG is also available from the Windows ***Start*** menu. You can pin DASIG to the *Start* menu or to the Windows Taskbar, like any other Windows application.

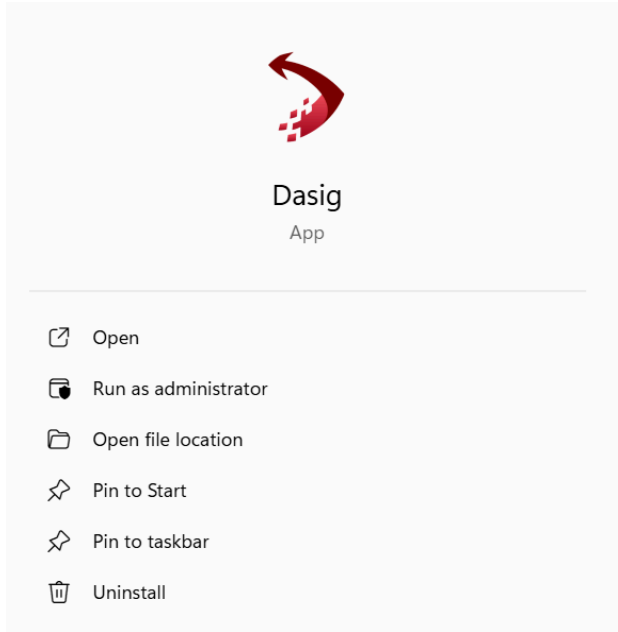


Figure 1.13. DASIG Application Available from the Windows Desktop and Start Menu

8. Troubleshooting

Issue: DASIG installer cannot be downloaded

Impact: The installer file cannot be saved to the local computer, preventing DASIG installation from proceeding.

Resolution: Institutional or secured networks may restrict the download of executable (.exe) files. If the DASIG installer cannot be downloaded, access the download link using an alternative network (e.g., a home or personal network). When prompted by the web browser, select Keep or Keep anyway to allow the installer file to be saved.

Issue: Browser security warnings block the installer

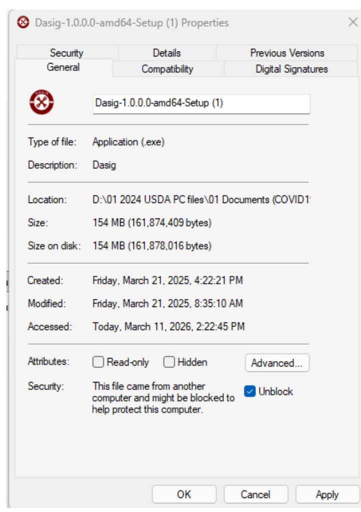
Impact: The DASIG setup file is blocked or removed by the web browser during download.

Resolution: Most web browsers display security warnings when downloading executable files. The wording and steps vary by browser (e.g., Google Chrome or Microsoft Edge). Follow the browser-specific prompt and select Keep or Keep anyway to retain the installer file.

Issue: Installation is blocked on institutional or managed computers

Impact: Installation cannot be completed due to system-level restrictions or insufficient user permissions.

Resolution: Installing DASIG for the current user only is recommended; however, local computer policies may still prevent installation. If installation fails or is blocked, contact local IT support staff to request installation assistance or temporary permissions. For US federal computers, remove the restriction by clicking the unblock button under PROPERTIES/GENERAL before installation.



Issue: Antivirus or security software prevents the installer from running

Impact: The DASIG setup file downloads successfully but does not launch or is immediately blocked during execution.

Resolution: Some antivirus or endpoint-protection programs restrict applications downloaded from the internet. Check whether security software is blocking the DASIG installer and consult the relevant documentation to allow or whitelist the installer, or temporarily permit execution during installation.

3. Sample Data File

   In the following chapters, the use of the DASIG model is demonstrated using example datasets that are installed automatically with the application. These files allow users to familiarize themselves with the workflow and functionality of each DASIG module before applying the model to their own data.

   The sample datasets can be accessed from the **Windows Start menu**. Open the Start menu, select **All** to display all installed applications, and navigate to the **Dasig Sample Datasets** folder, as shown in Figure 1.14.

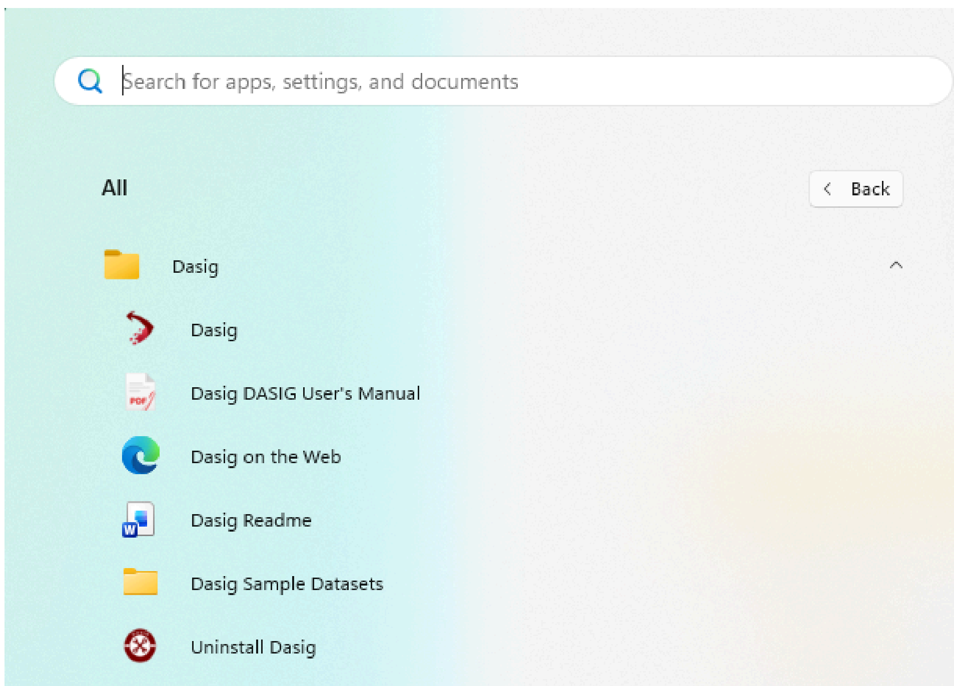


Figure 1.14. Accessing the DASIG Sample Datasets folder from the Windows Start menu.

The **Sample Datasets** directory contains several subfolders corresponding to the DASIG modules. These folders are organized in the same sequence in which the modules are introduced and discussed in this User Guide (Figure 1.15). Each folder contains example input files and outputs that are used in the corresponding chapter to illustrate module-specific procedures and expected results.

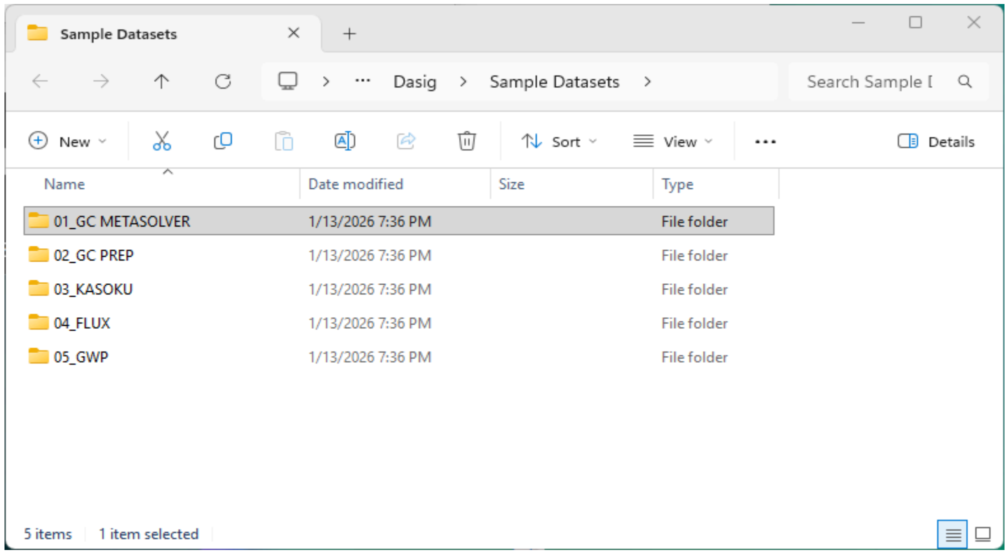


Figure 1.15. Organization of sample datasets by DASIG module.

IMPORTANT! The Sample Datasets folder is located within the DASIG application installation directory and can be found at the following locations, depending on the selected installation mode:

- for DASIG installed for the current user only: C:\users\<USERNAME>\AppData\Local\Programs\Dasig
- for DASIG installed for all users of the computer: C:\ProgramData\Dasig

Files located in these directories may be protected by Windows file permission settings. As a result, users may not be able to modify the original sample files directly. However, the files can be copied to any user-defined working directory where read/write permissions are available.

To avoid unintentional modification of the original datasets, users are encouraged to create their own working folders and use copies of the sample files for practice or analysis.

Chapter 2: GC Run Sequence Preparation Using GC Metasolver

1. Overview

Prior to GC analysis, gas sample identifiers and standard gas information are encoded using the **GC Metasolver** to generate a GC run sequence. GC Metasolver is a computational workbook designed to configure experimental units, define temporal sampling intervals, and execute randomized sequencing. The resulting randomization generates the GC run sequence, which programmatically specifies the sequence of sample injections. This run sequence defines the programmed order in which gas samples are injected, creating a batch that includes quality control standards, ambient air samples, and samples of unknown concentration.

The sequence of sample injections is randomized to ensure equal exposure of all samples to instrument sensitivity and to minimize systematic bias, thereby improving analytical reliability and data quality. In addition, check gas standards are inserted at regular intervals (typically every 10 samples) to evaluate detector performance and serve as independent quality control checks during GC analysis.

A separate run sequence file is prepared for each sampling date and saved as an Excel workbook. These run sequence files are subsequently used during GC operation to guide sample analysis.

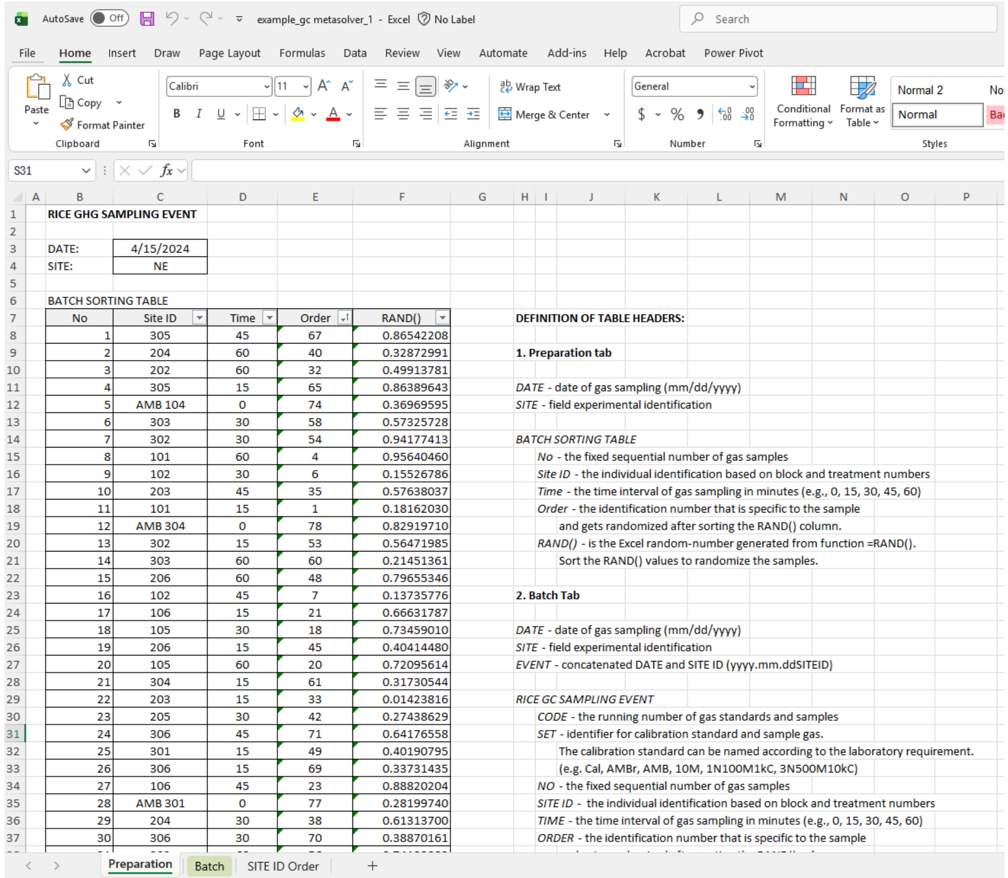
2. Quick Start

To create a GC run sequence script, users will use the GC Metasolver template, an Excel workbook provided with the DASIG installation. The template is located in the following directory:

Sample Datasets\01_GC Metasolver
The Sample Datasets folder can be accessed from the DASIG folder via the Windows Start menu.

1. Open the GC Metasolver template file, located at:
   Sample Datasets\01_GC Metasolver\gc metasolver template.xlsx

2. Select the *Preparation* tab. The user provides the following inputs:
   a. *DATE* field (column C3), type in the date of gas sampling following the format mm/dd/yyyy;
   b. *SITE* (C4) type in the field experimental identification or the field ID indicating where gas is collected (i.e. NE (Northeast experiment); GF1 (Greenfield experiment 1); RTVA (RiceTec varietal trial).


RICE GHG SAMPLING EVENT

DATE: 4/15/2024
SITE: NE

BATCH SORTING TABLE

No	Site ID	Time	Order	RAND()
1	305	45	67	0.86542208
2	204	60	40	0.32872991
3	202	60	32	0.49913781
4	305	15	65	0.86389643
5	AMB 104	0	74	0.36969595
6	303	30	58	0.57325728
7	302	30	54	0.94177413
8	101	60	4	0.95640460
9	102	30	6	0.15526786
10	203	45	35	0.57638037
11	101	15	1	0.18162030
12	AMB 304	0	78	0.82919710
13	302	15	53	0.56471985
14	303	60	60	0.21451361
15	206	60	48	0.79655346
16	102	45	7	0.13735776
17	106	15	21	0.66631787
18	105	30	18	0.73459010
19	206	15	45	0.40414480
20	105	60	20	0.72095614
21	304	15	61	0.31730544
22	203	15	33	0.01423816
23	205	30	42	0.27438629
24	306	45	71	0.64176558
25	301	15	49	0.40190795
26	306	15	69	0.33731435
27	106	45	23	0.88820204
28	AMB 301	0	77	0.28199740
29	204	30	38	0.61313700
30	306	30	70	0.38870161

DEFINITION OF TABLE HEADERS:

1. Preparation tab

DATE - date of gas sampling (mm/dd/yyyy)
SITE - field experimental identification

BATCH SORTING TABLE
No - the fixed sequential number of gas samples
Site ID - the individual identification based on block and treatment numbers
Time - the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60)
Order - the identification number that is specific to the sample and gets randomized after sorting the RAND() column.
RAND() - is the Excel random-number generated from function =RAND(). Sort the RAND() values to randomize the samples.

2. Batch Tab

DATE - date of gas sampling (mm/dd/yyyy)
SITE - field experimental identification
EVENT - concatenated DATE and SITE ID (yyyy.mm.ddSITEID)

RICE GC SAMPLING EVENT
CODE - the running number of gas standards and samples
SET - identifier for calibration standard and sample gas.
The calibration standard can be named according to the laboratory requirement. (e.g. Cal, AMBr, AMB, 10M, 1N100M1kC, 3N500M10kC)
NO - the fixed sequential number of gas samples
SITE ID - the individual identification based on block and treatment numbers
TIME - the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60)
ORDER - the identification number that is specific to the sample

Figure 2. 1. Example of the *Preparation* tab in the GC Metasolver file.

3. In the *BATCH SORTING TABLE*, the user produces a sample list containing the following inputs:
    a. *No* - the fixed sequential number of gas samples;
    b. *Site ID* - the individual identification based on block and treatment numbers (i.e. 101, 102);
    c. *Time* - the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60);
    d. *Order* - the identification number that is specific to the sample;
    e. *RAND()* - is the Excel random-number generated from function =RAND(). Sort the RAND() values to randomize the samples.

4. After setting the GC Metasolver inputs in the *Preparation* tab, randomize the samples using the *RAND()* values. After the randomization, *Site IDs* and its corresponding *Time* and *Order* will be rearranged. The *No.* dictates the running sequence number of the randomized samples and will be reflected in the *Batch* worksheet for cross-checking.

To ensure proper randomization, check for clustering or unintended patterns of the gas samples and verify even distribution of treatments across time intervals.

5. Select *Batch* tab. This worksheet reflects the GC run sequence of the gas samples based on the inputs provided in the *Preparation* worksheet and the results from the randomization.

   Details from the *Preparation* worksheet are referenced (cross-sheet referencing) or concatenated and will be automatically generated to the *Batch* worksheet based on the information entered in the *SET* cells. The following details should **NOT** be modified, specifically:

   a. *DATE* - (column E1) date of gas sampling (mm/dd/yyyy);
   b. *SITE* - (G1) field experimental identification;
   c. *EVENT* - (I1) concatenated DATE and SITE ID (yyyy.mm.ddSITEID);
   d. *CODE* - the running number of gas standards and samples;
   e. *No.* - (D4) the fixed sequential number of gas samples;
   f. *SITE ID* - (E4) the individual identification based on block and treatment numbers;
   g. *TIME* - (F4) the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60);
   h. *ORDER* - (G4) the identification number that is specific to the sample;
   i. *SAMPLE ID* (column I3) - concatenated ID containing the sampling *EVENT*

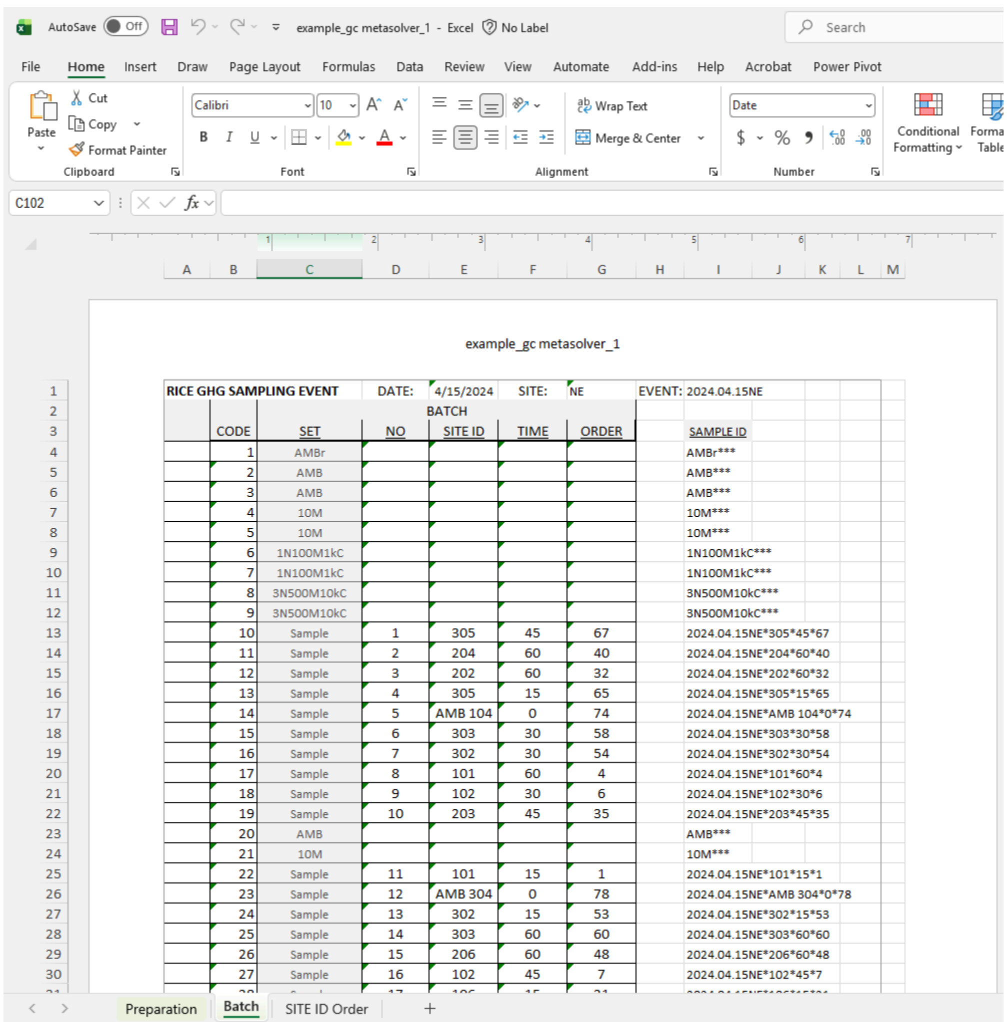
   The only cells or fields that will be **modified** by the user:

   i. *SET* - (C4) identifier for calibration 'standard' and 'sample' gas

      'Standard' - The calibration standard can be named according to the laboratory requirement (i.e. AMB, 10M, 1N100M1kC, 3N500M10kC, or AMBr; std).

      'Sample' - The user can only use '**Sample**' as an input in the cell. The worksheet will automatically cross-reference the *No.*, *Site ID*, *Time*, and *Order* from the *Preparation* worksheet. Concurrently, the *Code* (column B4) field is automatically generated, providing a sequential order and as the identifier assigned to all randomized gas samples, including the corresponding gas standards. This number is used for the sequence to arrange the gas samples and standards for GC analysis.

Note: The user can add gas standards before, in between, and after the set of gas samples. In this example, the set is organized such that the first ten entries correspond to the standard gases. These shall be followed by the sequence of gas samples. After every group of ten gas samples, an additional one or two standard gases shall be inserted. Upon completion of the gas-sample sequence, a final set of standard gases is appended to conclude the list.



1	RICE GHG SAMPLING EVENT		DATE:	4/15/2024	SITE:	NE	EVENT: 2024.04.15NE
2				BATCH			
3	CODE	SET	NO	SITE ID	TIME	ORDER	SAMPLE ID
4	1	AMBr					AMBr***
5	2	AMB					AMB***
6	3	AMB					AMB***
7	4	10M					10M***
8	5	10M					10M***
9	6	1N100M1kC					1N100M1kC***
10	7	1N100M1kC					1N100M1kC***
11	8	3N500M10kC					3N500M10kC***
12	9	3N500M10kC					3N500M10kC***
13	10	Sample	1	305	45	67	2024.04.15NE*305*45*67
14	11	Sample	2	204	60	40	2024.04.15NE*204*60*40
15	12	Sample	3	202	60	32	2024.04.15NE*202*60*32
16	13	Sample	4	305	15	65	2024.04.15NE*305*15*65
17	14	Sample	5	AMB 104	0	74	2024.04.15NE*AMB 104*0*74
18	15	Sample	6	303	30	58	2024.04.15NE*303*30*58
19	16	Sample	7	302	30	54	2024.04.15NE*302*30*54
20	17	Sample	8	101	60	4	2024.04.15NE*101*60*4
21	18	Sample	9	102	30	6	2024.04.15NE*102*30*6
22	19	Sample	10	203	45	35	2024.04.15NE*203*45*35
23	20	AMB					AMB***
24	21	10M					10M***
25	22	Sample	11	101	15	1	2024.04.15NE*101*15*1
26	23	Sample	12	AMB 304	0	78	2024.04.15NE*AMB 304*0*78
27	24	Sample	13	302	15	53	2024.04.15NE*302*15*53
28	25	Sample	14	303	60	60	2024.04.15NE*303*60*60
29	26	Sample	15	206	60	48	2024.04.15NE*206*60*48
30	27	Sample	16	102	45	7	2024.04.15NE*102*45*7

Figure 2.2. Example of the *Batch* tab in the GC Metasolver file.

6. Print the *Batch* worksheet to be used in arranging the gas samples and standards in the autosampler for GC analysis.

7. Select *SITE ID Order* tab. This worksheet contains *SITE ID* and the corresponding *TIME ID*. Additionally, the ambient gas sample (AMB) distributed accordingly to different set of SITE IDs and specified *TIME IDs* (i.e. AMB101 - t0).
   a. *SITE ID* - the individual identification based on block and treatment numbers which includes:
      1. Ambient gas sample collected in the field (e.g., AMB 101, AMB 104, AMB 201, AMB 204).
      2. Chamber identification number (e.g., 101, 102, 103, 201, 202, 203).
   b. *TIME ID* - the identification of the time interval during gas sampling (e.g., t0, t1, t2, t3, t4)

   The *SITE ID Order* input is highly needed for the DASIG-KASOKU module.

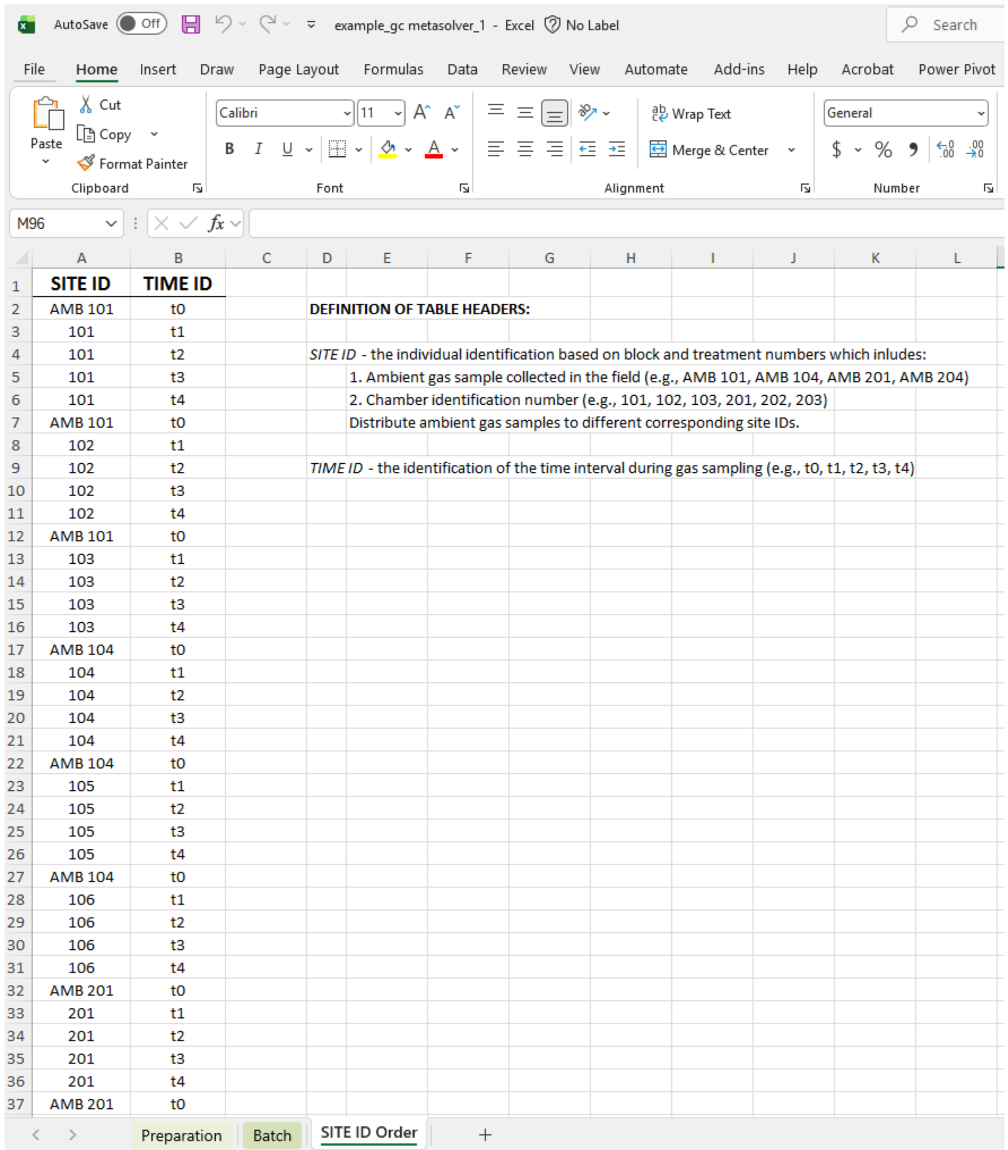


Figure 2.3. Example of the *Batch* tab in the GC Metasolver file.

8. Save the Excel workbook in a folder. Name your workbook based on the date of sampling, field ID and the type of file for traceability (i.e. 2025.04.12_NEprep, or 2025.04.12_NEgcmetasolver)

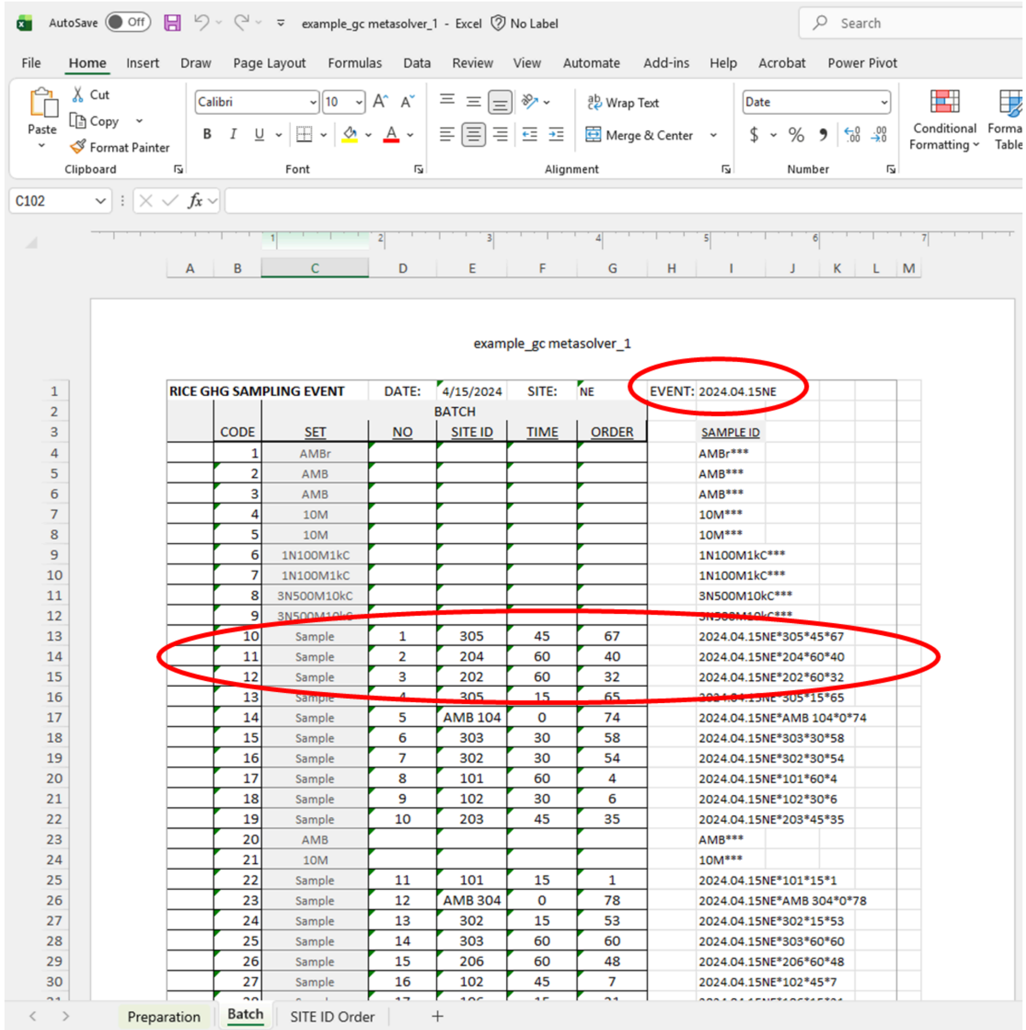
3. Input Specification

- In the *Preparation* tab, the experimental units (chamber ID) based on experimental design (blocks, treatments) should be provided correctly: *DATE* (day of gas sampling; mm/dd/yy), *SITE* (field ID), *Site ID* (individual identifier based on treatments and blocks), *Time* (time interval gas was collected), *Order* (sequential number) and *Rand()* (randomization value).

- In the *Batch* tab, the *SET* should be identified as ‘Sample’ or ‘Standard’. The other details in the worksheet will be generated automatically based on the input in the *SET* cells, and inputs from the *Preparation* worksheet.
- In the *SITE ID Order* tab, the *SITE IDs* are specific to the ambient field gas sample and its corresponding *TIME IDs*.

4. Tips to Optimal Procedure

- Use the GC Metasolver template file found in DASIG’s Sample Datasets folder to have uniform column headers and sheet names. This file will be used in the DASIG-KASOKU module.
- Verify if the input data from the *Preparation* tab is the same in the *Batch* and *SITE ID Order* tabs.
- Match the *Site IDs* and *Time IDs* columns in the *Preparation* tab to those in *SITE ID Order* tab. Moreover, the ambient field gas samples or t0 samples should be distributed to different *SITE ID*s accordingly.
- Check the *SAMPLE ID* column. The information should match the EVENT*NO*TIME*ORDER i.e. 2024.04.15NE*305*45*67 per sample.



example_gc metasolver_1

RICE GHG SAMPLING EVENT		DATE:	4/15/2024	SITE:	NE	EVENT:	2024.04.15NE
		BATCH					
CODE	SET	NO	SITE ID	TIME	ORDER		SAMPLE ID
1	AMBr						AMBr***
2	AMB						AMB***
3	AMB						AMB***
4	10M						10M***
5	10M						10M***
6	1N100M1kC						1N100M1kC***
7	1N100M1kC						1N100M1kC***
8	3N500M10kC						3N500M10kC***
9	3N500M10kC						3N500M10kC***
10	Sample	1	305	45	67		2024.04.15NE*305*45*67
11	Sample	2	204	60	40		2024.04.15NE*204*60*40
12	Sample	3	202	60	32		2024.04.15NE*202*60*32
13	Sample	4	305	15	65		2024.04.15NE*305*15*65
14	Sample	5	AMB 104	0	74		2024.04.15NE*AMB 104*0*74
15	Sample	6	303	30	58		2024.04.15NE*303*30*58
16	Sample	7	302	30	54		2024.04.15NE*302*30*54
17	Sample	8	101	60	4		2024.04.15NE*101*60*4
18	Sample	9	102	30	6		2024.04.15NE*102*30*6
19	Sample	10	203	45	35		2024.04.15NE*203*45*35
20	AMB						AMB***
21	10M						10M***
22	Sample	11	101	15	1		2024.04.15NE*101*15*1
23	Sample	12	AMB 304	0	78		2024.04.15NE*AMB 304*0*78
24	Sample	13	302	15	53		2024.04.15NE*302*15*53
25	Sample	14	303	60	60		2024.04.15NE*303*60*60
26	Sample	15	206	60	48		2024.04.15NE*206*60*48
27	Sample	16	102	45	7		2024.04.15NE*102*45*7

Figure 2.4. The *Batch* sheet in GC metasolver file.

- It is highly recommended to add the last set of standards in the *SET* in the *Batch* tab.

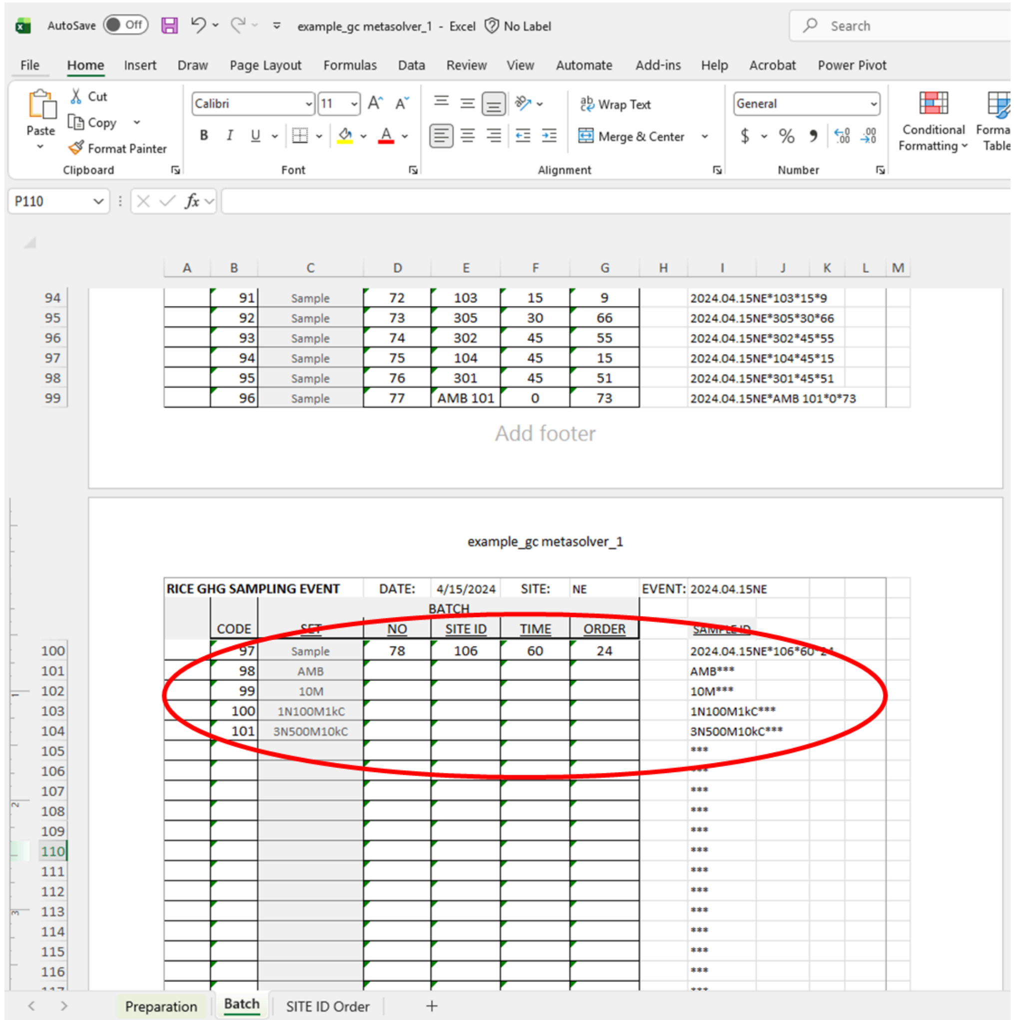


Figure 2.5. Standards are added after the last SITE ID.

- Once completed, name the GC Metasolver file based on the sampling date and format as date_SITEprep (i.e., 2025.04.15_NEprep) for ease in using the KASOKU module and traceability.

5. Troubleshooting

Issue: Inconsistent column headers, SITE IDs in Preparation tab and SITE ID order tab, and tab names.

Impact: The DASIG-KASOKU module fails to execute.

Resolution: **Use the GC metasolver template provided** for consistent names of columns and sheets. Check and verify the inputs are the same in all the GC metasolver workbook tabs.

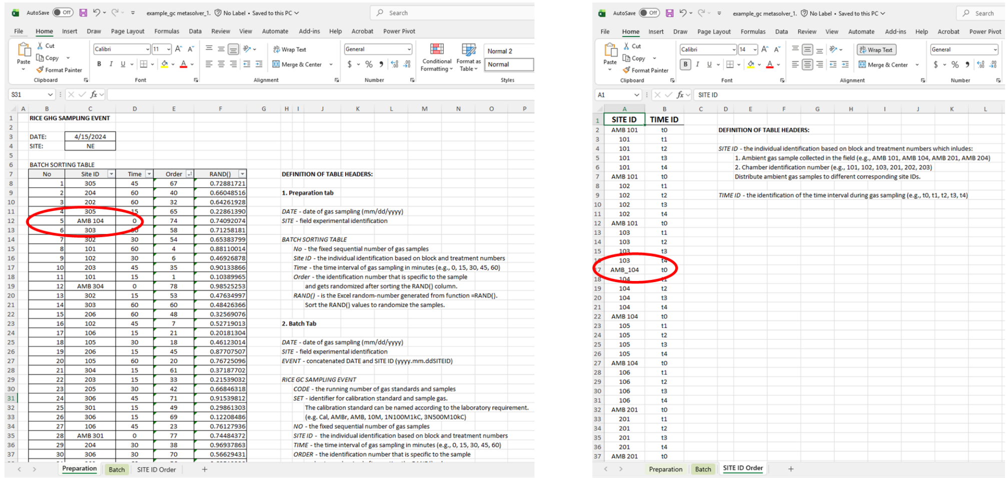


Figure 2.6. The information such as *SITE ID* and *TIME ID* in the *Preparation* tab match the *SITE ID Order* tab.

Issue:	Mismatch details or information of *SAMPLE ID* in the *Batch* tab.
Impact:	The DASIG-KASOKU module fails to execute.
Resolution:	The information should match the EVENT*NO*TIME*ORDER per sample.

Issue:	Inconsistent ambient field gas samples distribution in *SITE ID Order* tab.
Impact:	An error in sample identification, therefore the DASIG-KASOKU module fails to execute, or wrong outputs.
Resolution:	Verify the SITE IDs and TIME IDs based on the inputs in the *Preparation* tab and ambient field gas samples distribution.

6. Glossary

Term	Description
GC	Gas chromatography
GC Metasolver	An Excel worksheet used to prepare and generate the GC run sequence script prior to GC analysis. It is part of the DASIG model resources and contains fields for entering gas sampling date, site ID, batch information, and gas sample IDs to produce a randomized analytical sequence.

Preparation tab	A main tab within the GC metasolver file where users input required run parameters such as the *DATE*, *SITE*, *No.*, *Site ID*, *Time*, *Order*, and *Rand()* values .This serves as the starting point for creating the GC run sequence.
Batch tab	A supplementary tab within the GC Prep Datasheet file that is to generate and display the finalized batch run order, derived from the input and randomization performed in the Preparation tab.
SITE ID Order tab	A tab within the GC metasolver file where users input the SITE IDs, TIME IDs, and the distribution of ambient field gas samples (AMB) to specific sets of SITE IDs for the time interval 0 min.
DATE	Date of gas sampling (mm/dd/yyyy).
SITE	The field experimental identification.
No (NO)	The fixed sequential number of gas samples.
SITE ID (Site ID)	The individual identification based on block and treatment numbers.
Time (TIME)	the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60).
TIME ID	The identification of the time interval during gas sampling (e.g., t0, t1, t2, t3, t4)
Order (ORDER)	The identification number that is specific to the sample and gets randomized after sorting the RAND() column.
RAND() formula =RAND()	An Excel random-number generating function used in the Preparation tab to assign a random value to each gas sample entry. The generated random numbers are used to randomize the sample run order, minimizing measurement bias and improving the reliability of the GC analysis.

EVENT	The concatenated DATE and SITE ID (yyyy.mm.ddSITEID).
SET	The identifier for calibration standard and sample gas.
CODE	The running number of gas standards and samples.
SAMPLE ID	The concatenated ID contains the sampling EVENT, SITE ID, TIME and ORDER.

Chapter 3: DASIG-GC-PREP Module

1. Overview

The DASIG GC-PREP module automates the preprocessing of Shimadzu GC report files (Models 2014 and 2030). The module converts raw GC output files into standardized Peak Area Tables that are directly compatible with the DASIG-KASOKU module for subsequent concentration and flux calculations.

The GC-PREP module provides a modern, intuitive interface for importing, cleaning, merging, and organizing GC data. These automated workflows produce well-structured, analysis-ready datasets while substantially reducing manual data handling. By standardizing preprocessing steps across batches and sampling dates, GC-PREP improves consistency, traceability, and reproducibility of GC data preparation.

2. Quick Start

1. Select the working folder.
   Click the **Select Folder** button to specify a working directory for the GC-PREP module. This directory will serve as the primary output location where all generated files, including processed GC tables and intermediate results, will be saved.

   Users may select an existing folder or create a new folder as needed. It is recommended to use a dedicated project-specific directory to maintain clear organization of outputs.

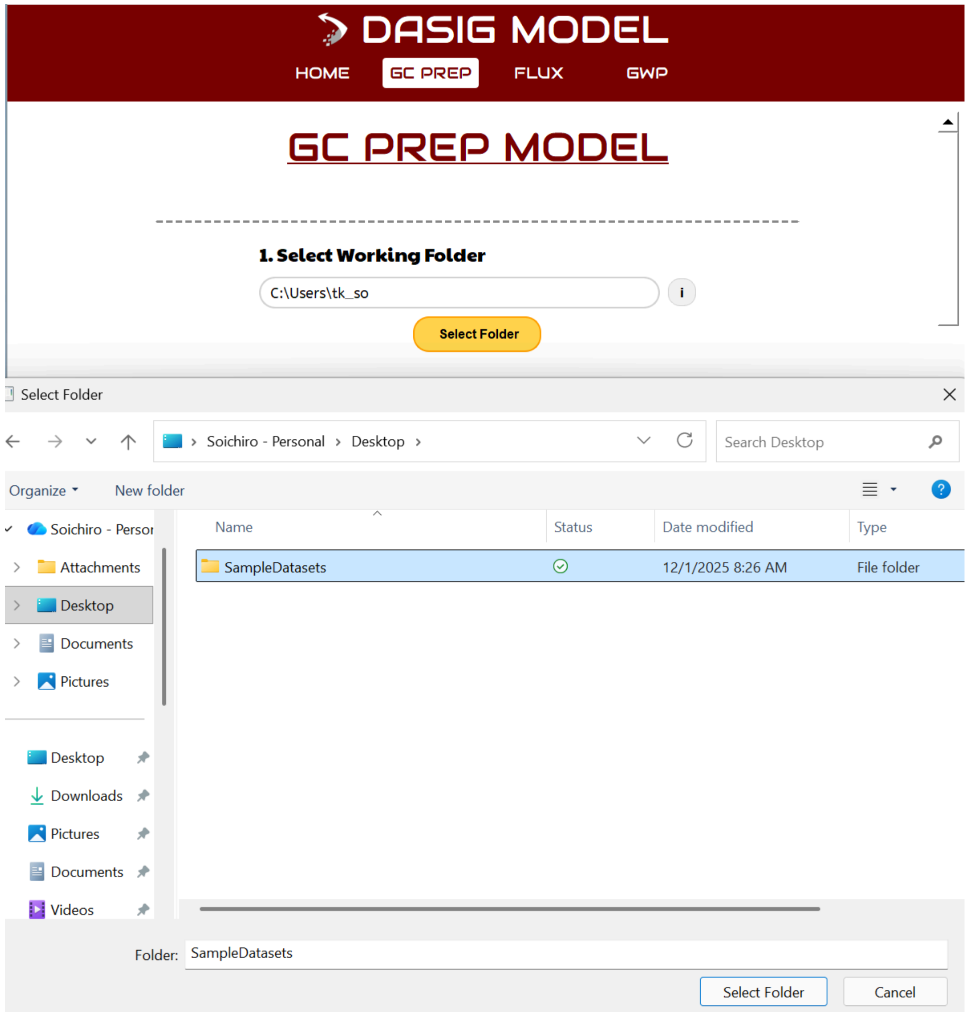


Figure 3.1. Selection of a working folder for GC-PREP output files.

2. Import GC report files.
   Drag and drop, or use “Open File”, to import one or more .txt report files generated byLabSolutions software of GC 2014 or 2030 models.

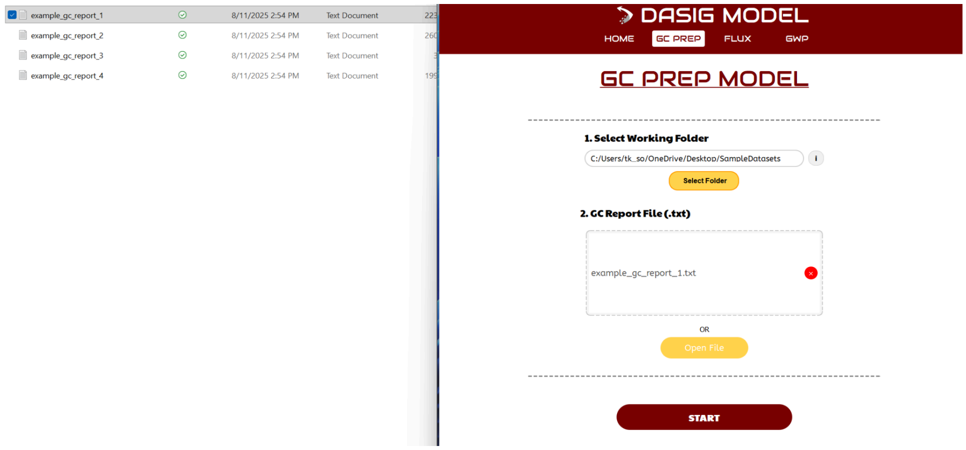


Figure 3.2. Drag and Drop (or Open) the Input File.

3. Run the module.
4. Review input files.
   Confirm file locations and metadata in the Input Review window.

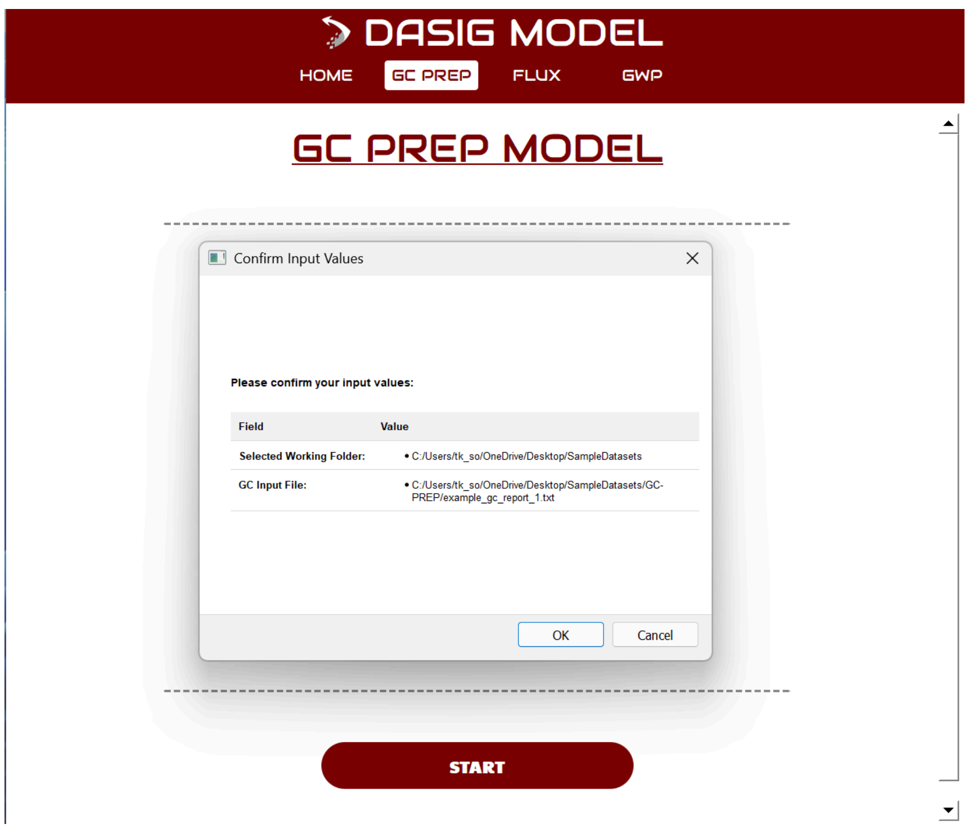


Figure 3.3 UI Inputs Confirmation Prompt.

5. Merge & reorder peaks.

Click on each file name to preview its data. If multiple files are imported, you may need to reorder the files using the date and time information. Select a file and drag it up or down to reorder.

Click *Merge* to create a unified table. Click *Next* when done.

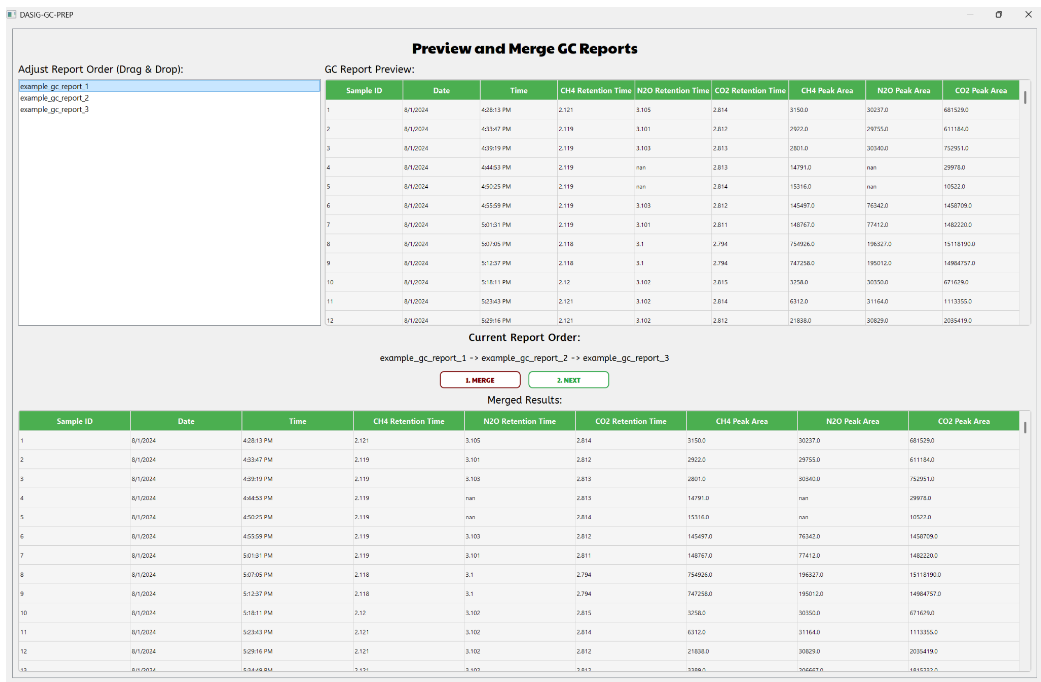
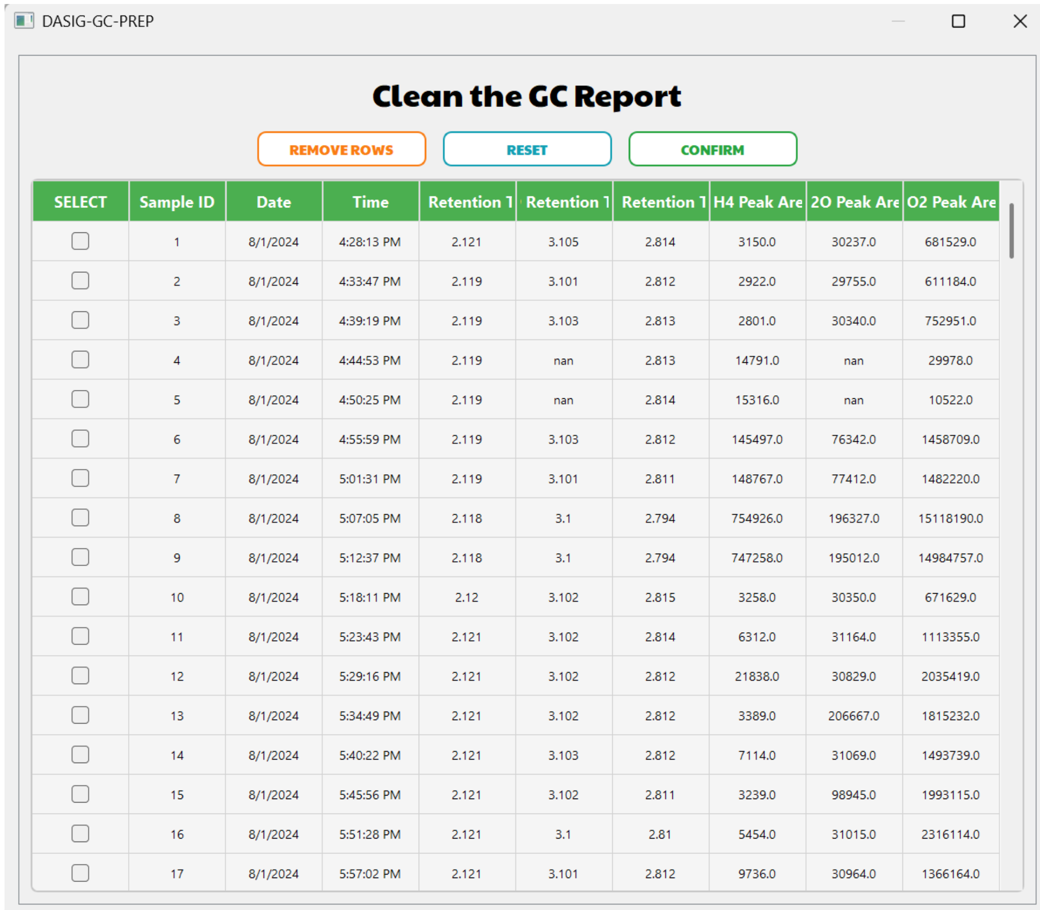


Figure 3.4. Merge Peak Tables Window.

6. Clean the table.
   Remove unwanted or irrelevant rows using the Clean Table step. GC report files may contain lines with content that must be removed. Select rows to be removed by clicking the corresponding check boxes. Click *Remove Rows* to remove the selected lines. You can use the *Reset* button to revert all editing. Press *Confirm* when done.



SELECT	Sample ID	Date	Time	Retention T	Retention T	Retention T	H4 Peak Are	2O Peak Are	O2 Peak Are
☐	1	8/1/2024	4:28:13 PM	2.121	3.105	2.814	3150.0	30237.0	681529.0
☐	2	8/1/2024	4:33:47 PM	2.119	3.101	2.812	2922.0	29755.0	611184.0
☐	3	8/1/2024	4:39:19 PM	2.119	3.103	2.813	2801.0	30340.0	752951.0
☐	4	8/1/2024	4:44:53 PM	2.119	nan	2.813	14791.0	nan	29978.0
☐	5	8/1/2024	4:50:25 PM	2.119	nan	2.814	15316.0	nan	10522.0
☐	6	8/1/2024	4:55:59 PM	2.119	3.103	2.812	145497.0	76342.0	1458709.0
☐	7	8/1/2024	5:01:31 PM	2.119	3.101	2.811	148767.0	77412.0	1482220.0
☐	8	8/1/2024	5:07:05 PM	2.118	3.1	2.794	754926.0	196327.0	15118190.0
☐	9	8/1/2024	5:12:37 PM	2.118	3.1	2.794	747258.0	195012.0	14984757.0
☐	10	8/1/2024	5:18:11 PM	2.12	3.102	2.815	3258.0	30350.0	671629.0
☐	11	8/1/2024	5:23:43 PM	2.121	3.102	2.814	6312.0	31164.0	1113355.0
☐	12	8/1/2024	5:29:16 PM	2.121	3.102	2.812	21838.0	30829.0	2035419.0
☐	13	8/1/2024	5:34:49 PM	2.121	3.102	2.812	3389.0	206667.0	1815232.0
☐	14	8/1/2024	5:40:22 PM	2.121	3.103	2.812	7114.0	31069.0	1493739.0
☐	15	8/1/2024	5:45:56 PM	2.121	3.102	2.811	3239.0	98945.0	1993115.0
☐	16	8/1/2024	5:51:28 PM	2.121	3.1	2.81	5454.0	31015.0	2316114.0
☐	17	8/1/2024	5:57:02 PM	2.121	3.101	2.812	9736.0	30964.0	1366164.0

Figure 3.5. Clean Peak Table Window.

7. Define Split Positions (if necessary).
   If necessary, the unified peak table can be split into separate datasets for processing. Specify where the merged table should be divided into separate files using the Split Table step. Click on a row to define the row that terminates a set. The next set starts on the row below the row selected. Observe the change in background colors to confirm the table is being split correctly.

   Note: If a table contains samples from different dates, table splitting is mandatory.

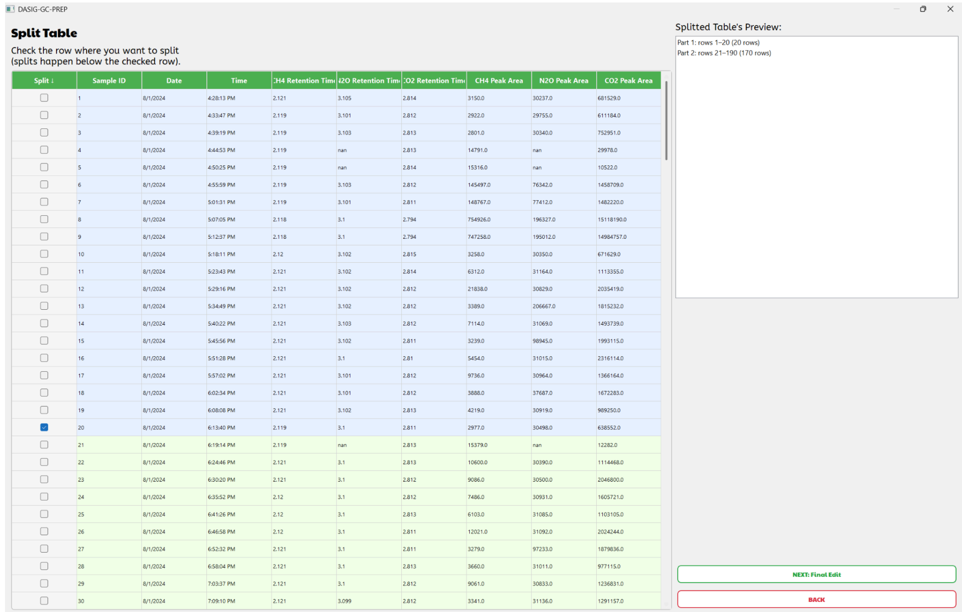


Figure 3.6. Split Peak Tables Window.

8. Final Review
   Inspect each resulting part for accuracy and completeness before export.

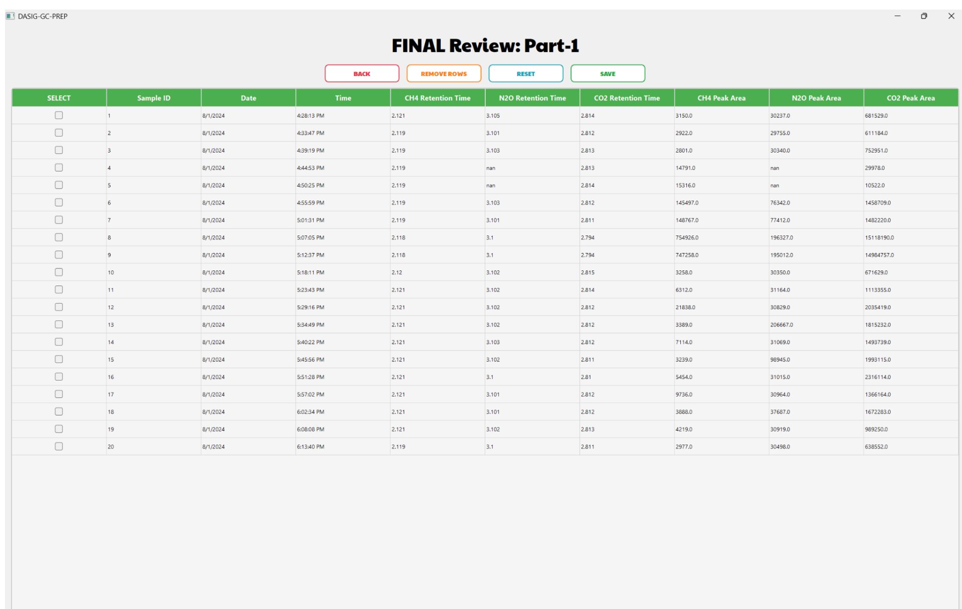


Figure 3.7. Final Review Window Per Splitted Peak Table Part.

9. Export Outputs
   Save proceeded Excel files such as part_1.xlsx and the default merged_output.xlsx into the designated output folder.

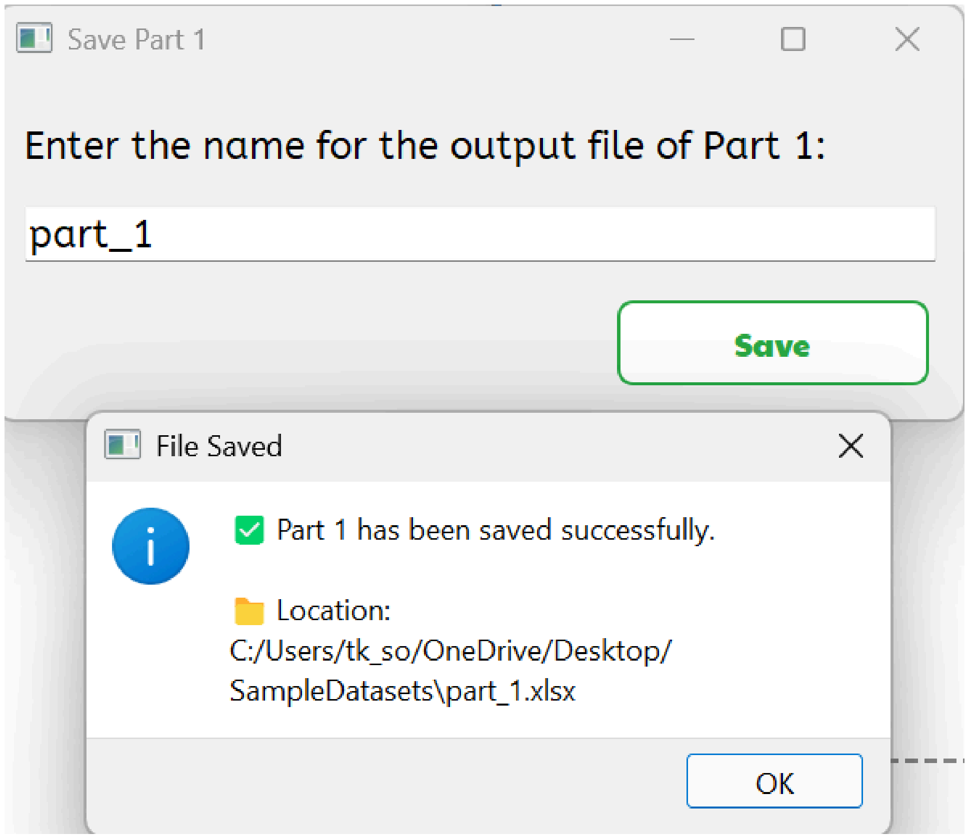


Figure 3.8. Naming Peak Table Part and Confirmation Window

3. Input Specification

The GC-PREP module requires as its input the output file in text (.txt) format generated by the Shimadzu GC 2014 or 2030 model with the LabSolutions software. Figure 3.9 shows an example of an output file exported from a Shimadzu LabSolutions in text (.txt) format.

```
[Header]
Application Name	LabSolutions
Version 5.111
Data File Name	C:\ORYZA GC DATA\GC DATA\002\ORYZA_NMC2_812024_1_001.gcd
Output Date	8/1/2024
Output Time	4:28:13 PM

[Configuration]
Instrument Name	ORYZA GC
Instrument #	3
Line #	1
# of Detectors	3
Detector ID	DET#1	DET#2	DET#3
Detector Name	FID	ECD	PTCD
# of Channels	1	1	1

[Peak Table(Ch1)]
# of Peaks	3
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Conc.	Mark	ID#	Name	k'	Plate #	Plate Ht.	Tailing	Resolution	Sep.Factor	Area Ratio	Height Ratio	Conc. %	Norm Conc.
1	1.934	1.882	2.068	2380	590	4.031	0.000		1	CO	0.000	5193	28.884	2.419	0.000	0.000	0	0	0.000	0.000
2	2.121	2.068	2.212	3150	1100	2.863	2.432	V	2	CH4	0.096	11607	12.923	1.130	2.006	0.000	0	0	0.542	0.542
3	2.814	2.735	3.158	681529	253515	2.688	446.632		3	CO2	0.455	22916	6.546	1.186	9.056	4.715	0	0	99.458	99.458

[Peak Table(Ch2)]
# of Peaks	1
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Conc.	Mark	ID#	Name	k'	Plate #	Plate Ht.	Tailing	Resolution	Sep.Factor	Area Ratio	Height Ratio	Conc. %	Norm Conc.
1	3.105	3.032	3.258	30237	7643	3.956	0.277		1	N2O	0.000	13498	11.113	1.302	0.000	0.000	0	0	100.000	100.000

[Peak Table(Ch3)]
# of Peaks	0

[Header]
Application Name	LabSolutions
Version 5.111
Data File Name	C:\ORYZA GC DATA\GC DATA\002\ORYZA_NMC2_812024_2_002.gcd
Output Date	8/1/2024
Output Time	4:33:47 PM

[Configuration]
Instrument Name	ORYZA GC
Instrument #	3
Line #	1
# of Detectors	3
Detector ID	DET#1	DET#2	DET#3
```

Figure 3.9. Example of output file from Shimadzu LabSolutions in text format.

This input file must be structured into the following data sections:

- [Header]
  Contains general metadata such as Data File Name, Output Data, and Output Time.
- [Configration]
  Includes measurement and method parameters used during the GC analysis.
- [Peak Table(Ch1)] through [Peak Table(Ch3]
  Provides peak detection and qualification results for each GC channel, including retention time, peak area, and related analytical values.

The GC-PREP module parses these sections sequentially to extract the necessary analytical data for downstream processing and modeling.

4. Tips to Optimal Procedure

- Organize LabSolutions report files prior to import.
  Place all LabSolutions text (.txt) report files for a given analytical batch within the same working directory before importing into GC-PREP module.
- Ensure LabSolutions reports are complete.
  Each report must include the **Heade**r, **Configuration**, and **Peak Table** sections. Incomplete reports may trigger warnings during GC-PREP processing.

- Import related GC runs together.
  Upload files from the same sampling date or analytical run. This maintains dataset continuity.
- Review the *Input Confirmation* window carefully.
  Verify that all intended .txt files are listed and that filenames correspond to the correct run before proceeding.
- Remove non-data rows during the *Clean Table* step.
  Delete blank rows, and non-sample entries at this stage to prevent propagation of unwanted data into exported tables.
- Apply *Split Table* only when required.
  Use splitting when the merged dataset intentionally contains multiple sampling dates or processing batches that must be exported separately.
- Complete a *Final Review* before exporting.
  Confirm that CH_4, N_2O, and CO_2 peaks appear in the correct columns, sample identifiers are intact, and record count matches expectations.
- Retain all original GC text files.
  GC-PREP module does not modify imported .txt files. These files should be archived as the primary audit reference.
- Maintain clear naming convention of exported files.
  Default GC-PREP output filenames (e.g., merged_output.xlsx, part_1.xlsx) are recommended to preserve workflow traceability.
- Document any manual cleaning actions.
  If peaks are removed or corrected during *Clean Table* or *Final Review*, brief notes are recommended for QA/QC documentation.
- Processed files may be re-loaded if adjustments are required.
  GC-PREP output files can be imported back into the module to repeat cleaning, merging, or splitting steps without recreating inputs.

5. Model Processing Flow

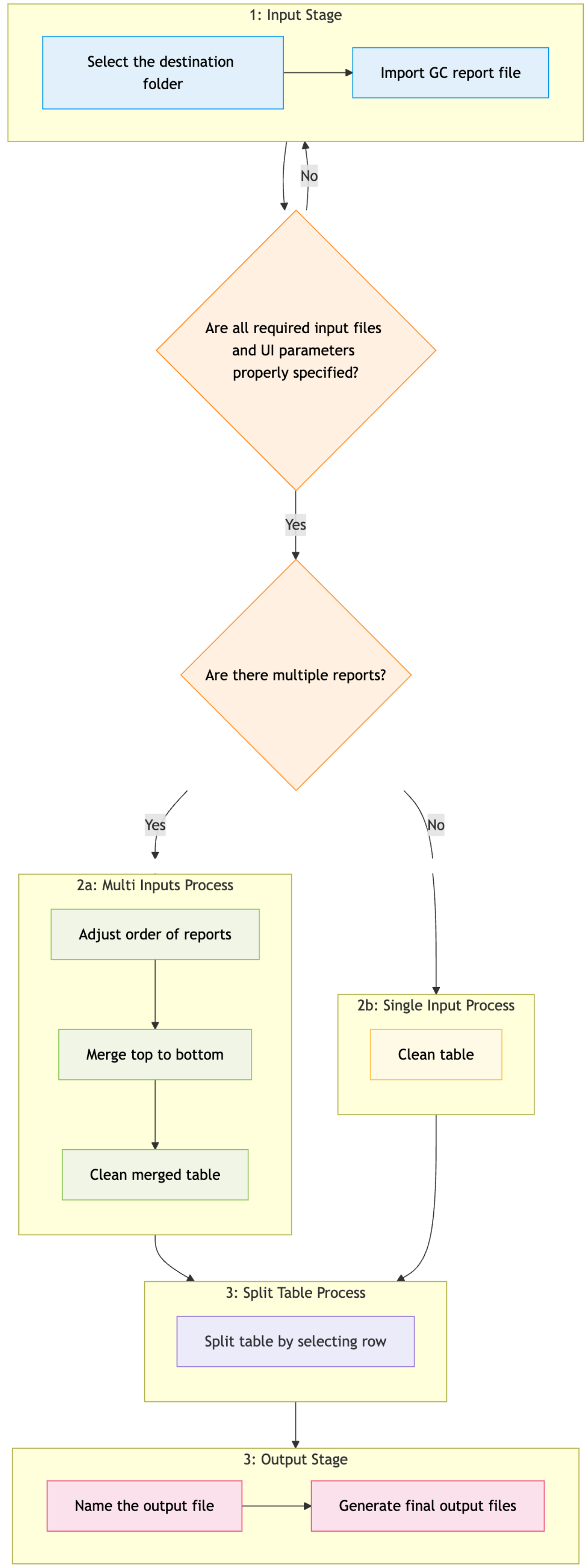


Figure 3.10. Flow diagram representing the core processing phases.

6. Quality Assurance / Quality Control (QA/QC)

The GC-PREP module implements an integrated QA/QC framework to ensure data integrity, consistency, and analytical reliability across the entire data processing workflow.

- *Input Data Interpretation*:
  Structured .txt files exported from Shimadzu LabSolutions are automatically interpreted and converted into standardized tabular datasets. Each record represents a unique GC measurement, maintaining one-to-one traceability between input and output data.
- *Gas Identification*:
  Gas identification is performed using an internal alias-matching system operating in a case-insensitive manner, ensuring consistent recognition of gas species regardless of naming validations in the source files.
- *Parameter Extraction*:
  For each detected gas, key analytical parameters, including Retention Time and Peak Area are extracted and validated during processing.
- *Output Standardization*:
  All generated datasets conform to a fixed and consistent column sequence, ensuring compatibility with downstream analytical tools, models, and reporting pipelines.
- *Sequential Integrity Check*:
  Sequential numbering of records is validated to detect duplication, omission, or ordering inconsistencies during data processing.
- *Traceability of Data Processing*:
  All data parsing, cleaning, and splitting operations are designed to be fully traceable, supporting reproducibility, audit readiness, and transparent data lineage.
- *Output Compliance*:
  Final output files are validated to ensure compliance with DASIG analytical data standards, confirming their suitability for downstream analysis and long-term data management.

7. Output Interpretation

Table 3.1. GC-PREP output files and their descriptions.

Output Item	**Description**
part_1.xlsx, *part_2*.xlsx,	Individual report segments after

…	processing. The <PartName> portion is user-defined or system-assigned during the processing step.

	A	B	C	D	E	F	G	H	I
1	Sample ID	Date	Time	CH4 Retention Time	N2O Retention Time	CO2 Retention Time	CH4 Peak Area	N2O Peak Area	CO2 Peak Area
2	1	8/1/2024	4:28:13 PM	2.121	3.105	2.814	3150.0	30237.0	681529.0
3	2	8/1/2024	4:33:47 PM	2.119	3.101	2.812	2922.0	29755.0	611184.0
4	3	8/1/2024	4:39:19 PM	2.119	3.103	2.813	2801.0	30340.0	752951.0
5	4	8/1/2024	4:44:53 PM	2.119	nan	2.813	14791.0	nan	29978.0
6	5	8/1/2024	4:50:25 PM	2.119	nan	2.814	15316.0	nan	10522.0
7	6	8/1/2024	4:55:59 PM	2.119	3.103	2.812	145497.0	76342.0	1458709.0
8	7	8/1/2024	5:01:31 PM	2.119	3.101	2.811	148767.0	77412.0	1482220.0
9	8	8/1/2024	5:07:05 PM	2.118	3.1	2.794	754926.0	196327.0	15118190.0
10	9	8/1/2024	5:12:37 PM	2.118	3.1	2.794	747258.0	195012.0	14984757.0
11	10	8/1/2024	5:18:11 PM	2.12	3.102	2.815	3258.0	30350.0	671629.0
12	11	8/1/2024	5:23:43 PM	2.121	3.102	2.814	6312.0	31164.0	1113355.0
13	12	8/1/2024	5:29:16 PM	2.121	3.102	2.812	21838.0	30829.0	2035419.0
14	13	8/1/2024	5:34:49 PM	2.121	3.102	2.812	3389.0	206667.0	1815232.0
15	14	8/1/2024	5:40:22 PM	2.121	3.103	2.812	7114.0	31069.0	1493739.0
16	15	8/1/2024	5:45:56 PM	2.121	3.102	2.811	3239.0	98945.0	1993115.0
17	16	8/1/2024	5:51:28 PM	2.121	3.1	2.81	5454.0	31015.0	2316114.0
18	17	8/1/2024	5:57:02 PM	2.121	3.101	2.812	9736.0	30964.0	1366164.0
19	18	8/1/2024	6:02:34 PM	2.121	3.101	2.812	3888.0	37687.0	1672283.0
20	19	8/1/2024	6:08:08 PM	2.121	3.102	2.813	4219.0	30919.0	989250.0
21	20	8/1/2024	6:13:40 PM	2.119	3.1	2.811	2977.0	30498.0	638552.0
22	21	8/1/2024	6:19:14 PM	2.119	nan	2.813	15379.0	nan	12282.0
23	22	8/1/2024	6:24:46 PM	2.121	3.1	2.813	10600.0	30390.0	1114468.0
24	23	8/1/2024	6:30:20 PM	2.121	3.1	2.812	9086.0	30500.0	2046800.0
25	24	8/1/2024	6:35:52 PM	2.12	3.1	2.812	7486.0	30931.0	1605721.0
26	25	8/1/2024	6:41:26 PM	2.12	3.1	2.813	6103.0	31085.0	1103105.0
27	26	8/1/2024	6:46:58 PM	2.12	3.1	2.811	12021.0	31092.0	2024244.0
28	27	8/1/2024	6:52:32 PM	2.121	3.1	2.811	3279.0	97233.0	1879836.0
29	28	8/1/2024	6:58:04 PM	2.121	3.1	2.813	3660.0	31011.0	977115.0
30	29	8/1/2024	7:03:37 PM	2.121	3.1	2.812	9061.0	30833.0	1236831.0
31	30	8/1/2024	7:09:10 PM	2.121	3.099	2.812	3341.0	31136.0	1291157.0
32	31	8/1/2024	7:14:43 PM	2.121	3.098	2.813	10600.0	30992.0	1098103.0
33	32	8/1/2024	7:20:16 PM	2.118	3.096	2.81	149308.0	78894.0	1476680.0
34	33	8/1/2024	7:25:49 PM	2.121	3.098	2.811	3376.0	31185.0	2230632.0
35	34	8/1/2024	7:31:23 PM	2.121	3.098	2.812	10545.0	32000.0	1721358.0
36	35	8/1/2024	7:36:55 PM	2.121	3.099	2.813	3408.0	31066.0	646512.0
37	36	8/1/2024	7:42:29 PM	2.121	3.099	2.813	5971.0	31102.0	1139218.0
38	37	8/1/2024	7:48:01 PM	2.12	3.1	2.811	10130.0	31002.0	1982181.0

Figure 3.11. Example Output File (.xlsx) from the DASIG-GC-PREP Module

Table 3.2. GC-PREP output column definitions.

Column	Description
Sample ID	Unique identifier assigned to each GC measurement sample
Date	Analysis date recorded by the GC system
Time	Analysis start time recorded by the GC system
Retention Time (CH_4, N_2O, CO_2)	Retention time for each target gas, measured in minutes. This dataset evaluates GC and column performance.
Peak Area (CH_4, N_2O, CO_2)	Integrated peak area for each target gas, used for quantitative analysis

8. Troubleshooting

Issue: GC report file cannot be imported
Impact: The GC-PREP module cannot proceed because the selected file is not recognized as a valid Shimadzu LabSolutions report. No peak tables are generated.
Resolution: Ensure that the input file is a raw text (.txt) output exported directly from Shimadzu LabSolutions (Models 2014 or 2030). Confirm that the file contains the required sections, including [Header], [Configuration], and [Peak Table] blocks. Re-export the report from LabSolutions if necessary.

Issue: One or more imported files appear incomplete or empty
Impact: Merged peak tables may be misaligned by date or sequence, potentially affecting downstream processing.
Resolution: Use the Merge & Reorder Peaks step to manually reorder files \ based on sampling date and time before merging. Confirm the sequence visually in the preview pane prior to clicking Merge.

Issue: Unwanted rows appear in the merged peak table
Impact: Non-sample rows (e.g., blanks, headers, or instrument notes) may propagate into exported Excel files and interfere with downstream analysis.
Resolution: Use the Clean Table step to remove irrelevant or non-data rows. Review selections carefully and use the Reset option if unintended rows are removed.

Issue: Incorrect table splitting or missing split points
Impact: Output files may combine multiple sampling dates or analytical batches that should be processed separately.
Resolution: Apply the Split Table step when datasets contain multiple sampling dates or logical groupings. Confirm split boundaries by checking background color changes and reviewing each resulting table during the Final Review step.

Issue: Exported Excel files do not match expected structure
Impact: Downstream modules (e.g., DASIG-KASOKU) may reject the files or generate errors during processing.
Resolution: Before exporting, verify during Final Review that retention

times and peak areas for CH_4, N_2O, and CO_2 are correctly populated, sample identifiers are intact, and the number of records matches expectations.

Issue: Need to revise or repeat preprocessing steps

Impact: Users may be unsure whether the entire workflow must be repeated from the beginning.

Resolution: Previously exported GC-PREP Excel files can be re-imported into the module for additional cleaning, merging, or splitting without reloading the original LabSolutions reports.

9. Glossary

Term	Definition
Shimadzu GC 2014/2030	Gas chromatograph model manufactured by Shimadzu, supported as an input source for DASIG-GC-PREP preprocessing.
Shimadzu LabSolutions	Shimadzu's chromatography data system used to generate GC analysis reports and raw output files.
LabSolutions Report Files (raw .txt outputs)	Text-based GC report files exported from Shimadzu LabSolutions, used as input files for the DASIG-GC-PREP module.
Peak Area Tables	Structured tabular datasets generated from raw GC outputs generated by GC-PREP module, containing retention times and peak areas for target gases. This is the input file for the KASOKU module.
Clean Table Step	A preprocessing step in DASIG-GC-PREP that removes irrelevant entries and standardizes data structure prior to splitting.
Split Table Step	A preprocessing step in DASIG-GC-PREP that divides cleaned datasets into logical parts for individual report generation.
DASIG Analytical Data Standards	Internal data standards that define formatting, structure, and quality requirements for analytical data within the DASIG model.

Chapter 4: DASIG-KASOKU Module

1. Overview

The DASIG KASOKU module calculates optimal linear calibration parameters (slope and intercept) to convert peak areas into gas concentrations (ppm) for CH_4, CO_2, and N_2O. It uses Peak Areas Table and GC Metasolver as input files.

To ensure accuracy, the module evaluates all standard–peak combinations and filters them by coefficient of variance (CV) $\leq 3\%$ (default or user-defined). Linear calibration curves are then generated, and only those achieving $R^2 \geq 0.996$ (default) are accepted, unless alternative R^2 thresholds are specified. The selected curve provides the final calibration parameters applied to compute sample concentrations.

For transparency and documentation, the module outputs regression plots for each gas, embedded within the result file and saved as standalone images.

2. Quick Start

1. Name the Output Folder.
   Create an output folder where all generated files will be saved.

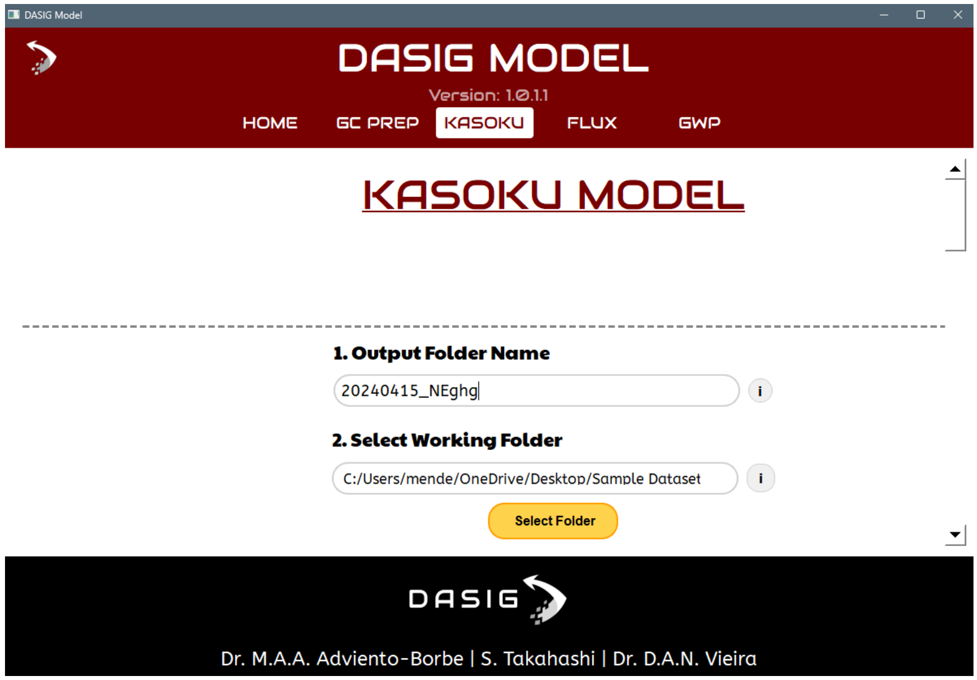


Figure 4.1. Kasoku Model Interface for Output and Working Folder Identification.

2. Specify the Working folder.
   Click the *Select Folder* button to designate a working folder for storing the output folder. If no working folder is specified, the home directory will be used by default.

3. Name the Output file.
   Specify a file name for the Kasoku output file. If this field is left blank, the model will apply the default name *"kasoku_output"*. The output will be saved in .xlsx format.

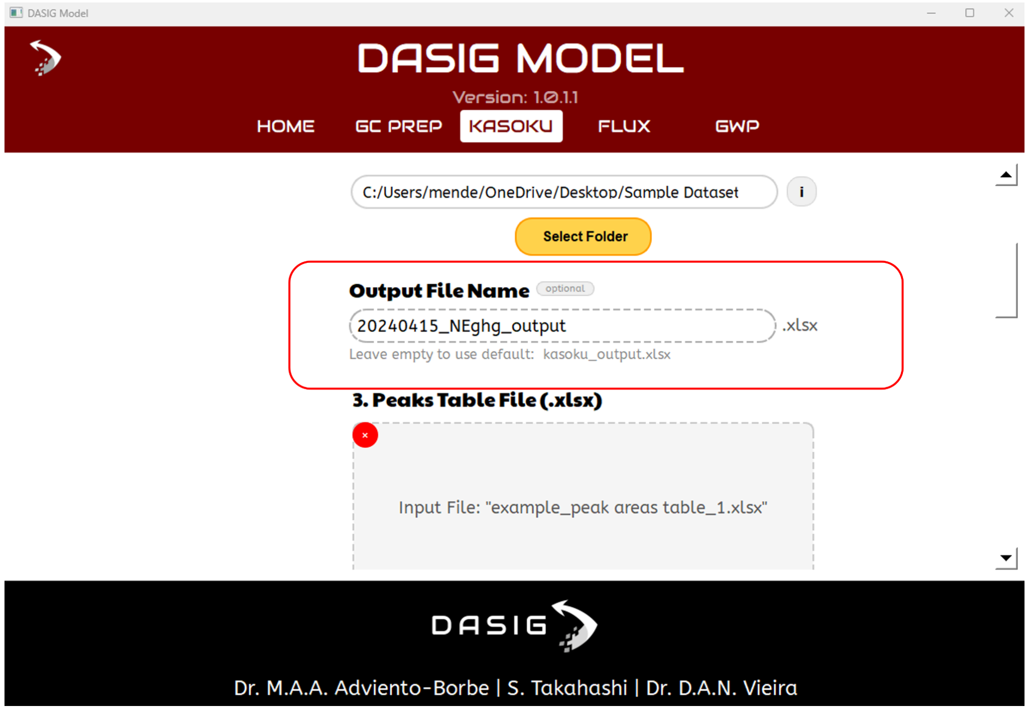


Figure 4.2. Output File Naming Interface in the Kasoku Module.

4. Import Input Files.
   Use the *Open File* buttons to upload the required Peaks Table File (.xlsx) and Preparation File (.xlsx) separately.

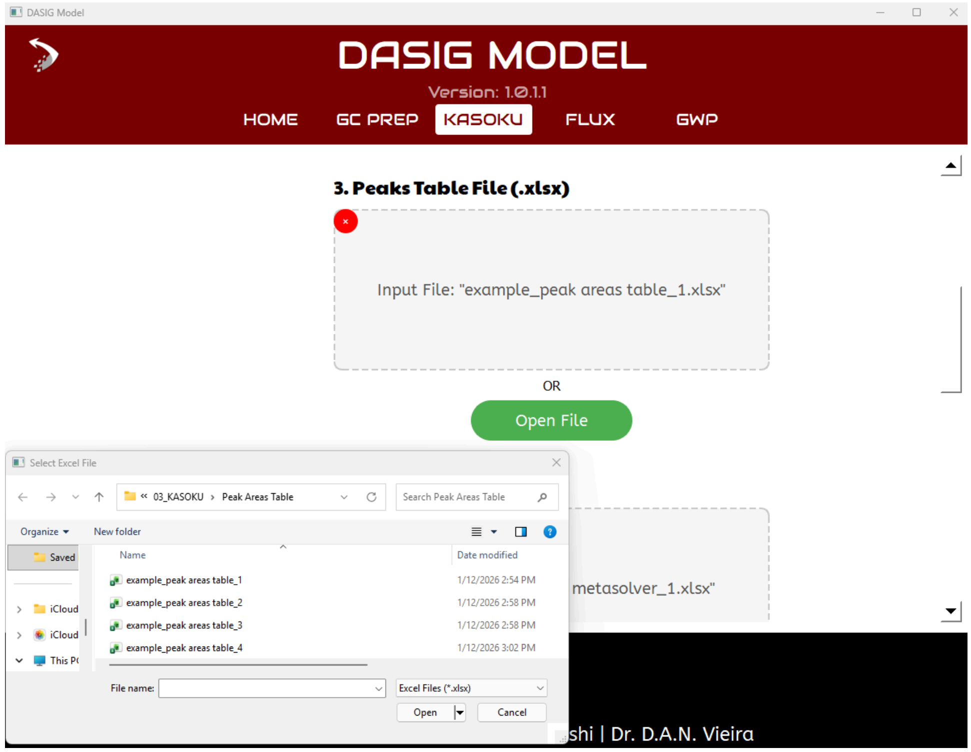


Figure 4.3. User Interface for Selecting the Peak Areas Table (.xlsx) in Kasoku Model.

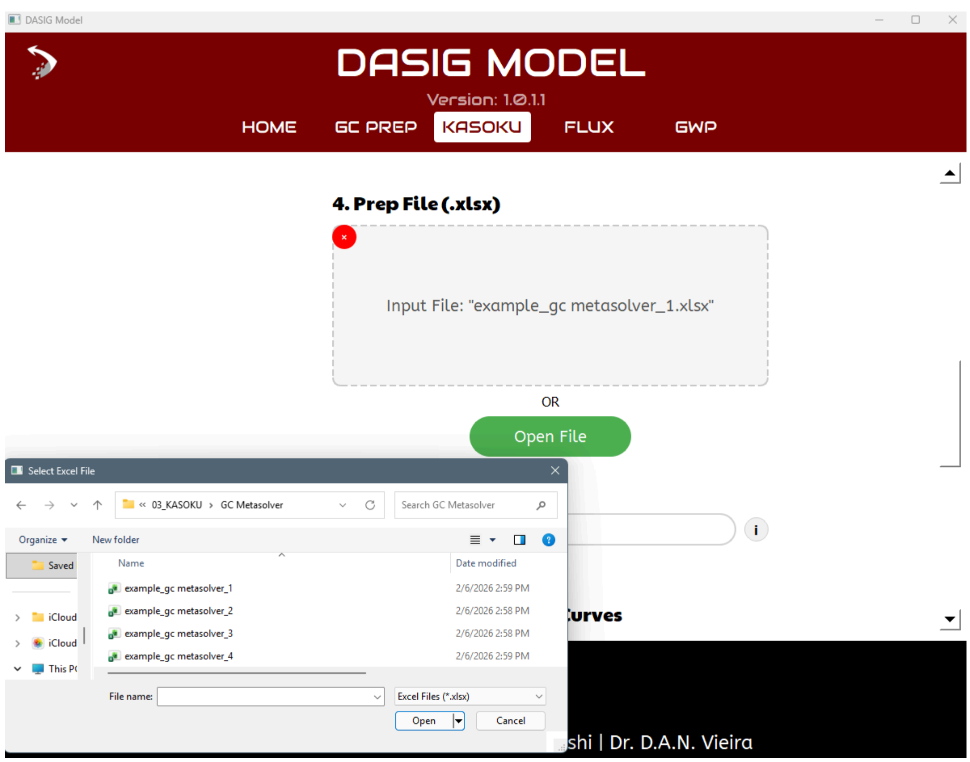


Figure 4.4. User Interface for Uploading the GC Metasolver (.xlsx) File.

5. Configure Thresholds.
   Specify the CV threshold (default by 3%) and identify the standard gas peaks to be used for calibration. Set the R^2 threshold (default by ≥ 0.996) for all trace gases.

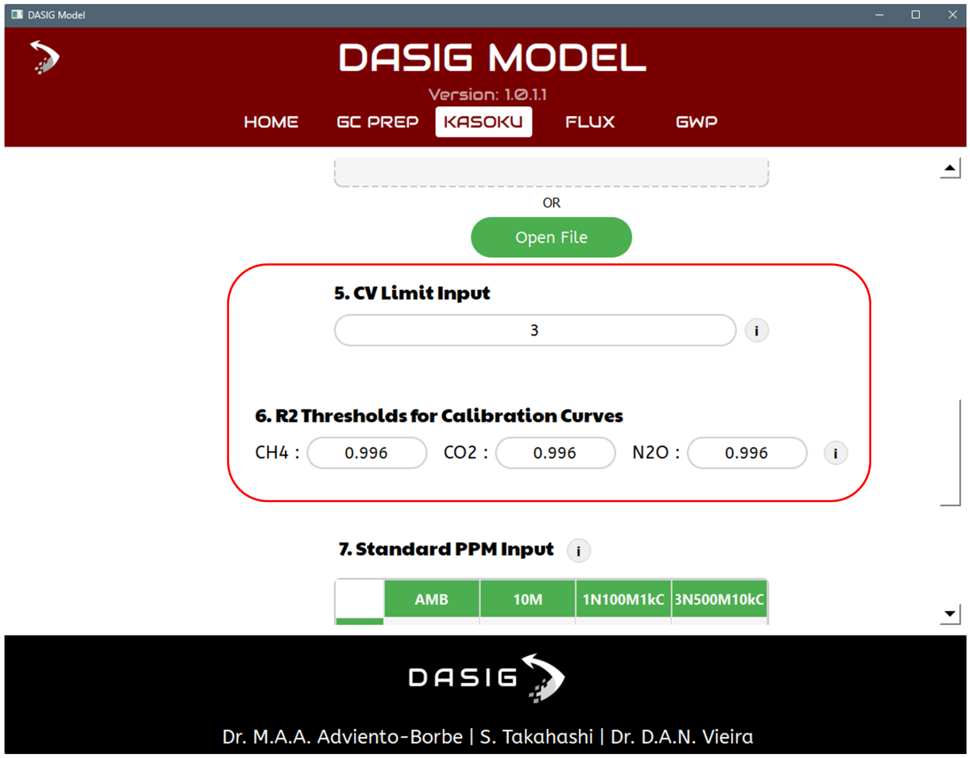


Figure 4.5. User Input Panel for CV Limits and R^2 Threshold Configuration.

6. Enter the individual concentrations of CH_4, N_2O, and CO_2 from each standard gas (AMB, 10M, 1N100M1kC, and 3N500M10kC) for calibration.

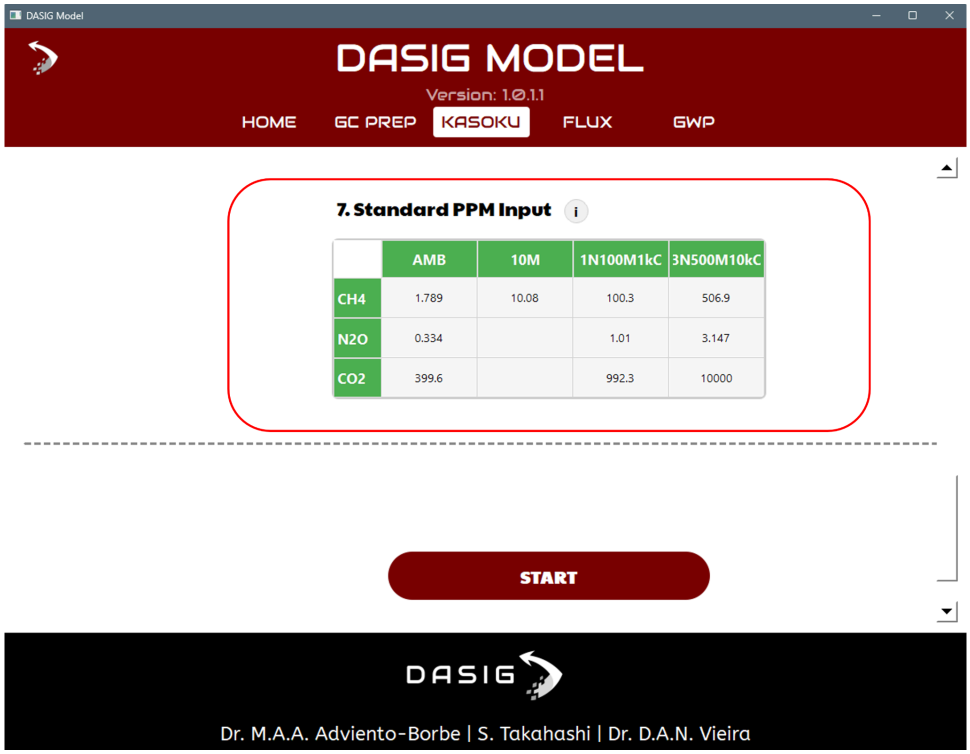


Figure 4.6. Standard Gas Concentration Input Table for CH_4, N_2O, and CO_2.

7. Run the Module.
   Click the *START button* to evaluate peak-standard combinations and generate calibration curves. Confirm all input values displayed in the pop-up dialog by clicking *OK*. If any value is incorrect, click *CANCEL* and update all input fields as needed before proceeding.

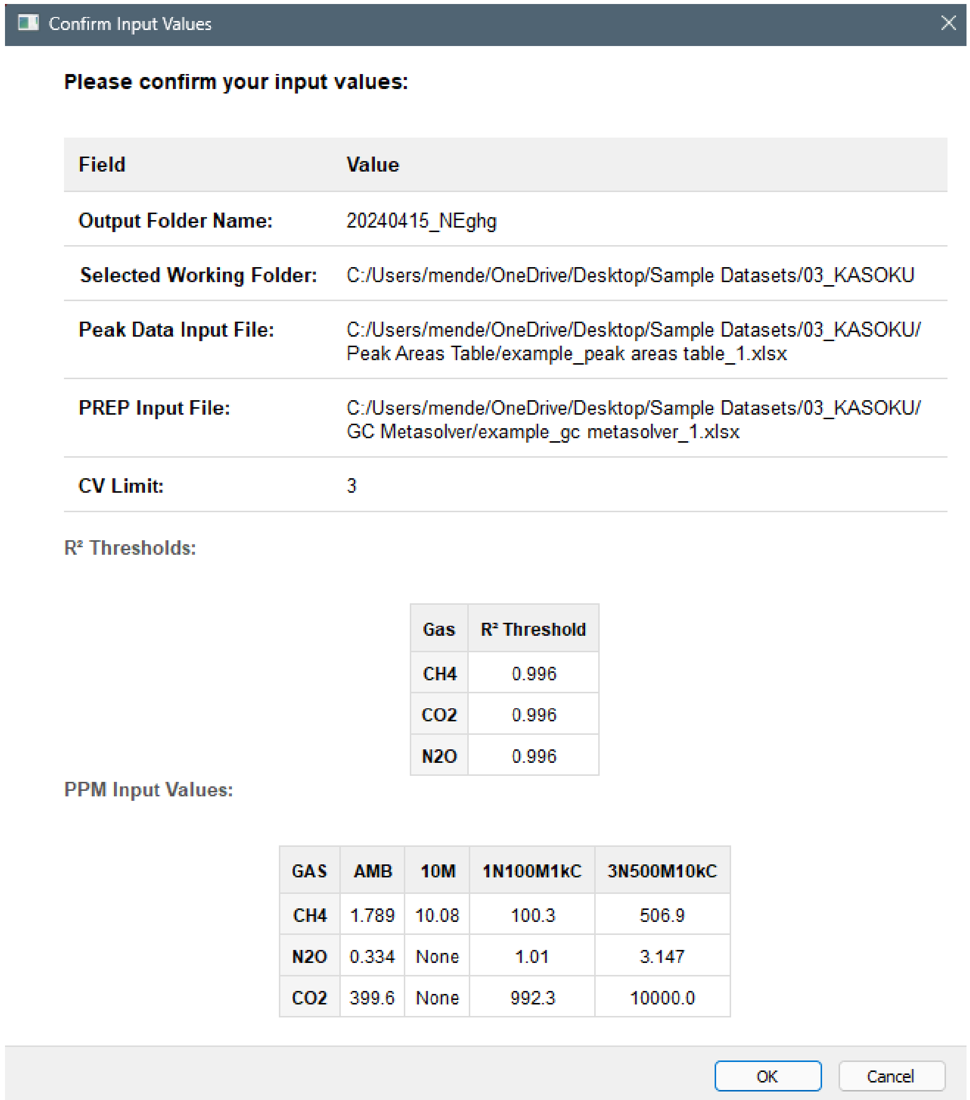


Figure 4.7. Kasoku Model Input Values Confirmation Prompt.

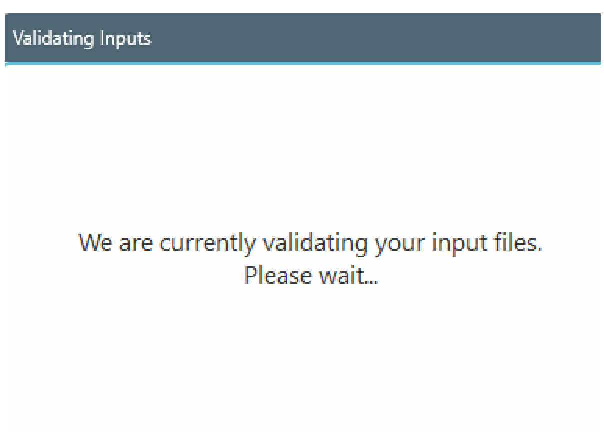


Figure 4.8. Input Validation Status Screen.

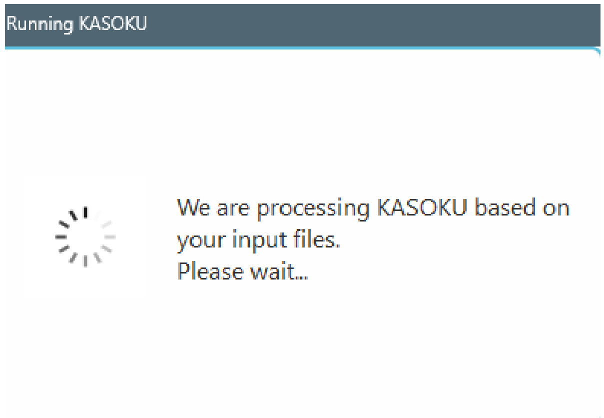


Figure 4.9. Kasoku Model Run Status Screen

8. Quality Control Handling.
    a. If no combination meets both the CV and R^2 criteria, the module stops after producing the QA/QC sheet and does not proceed to calibration curves and concentration calculation.
    b. If valid combinations exist, the module continues through calibration curves and concentration computation.

9. Export Outputs
   All results, including calibration plots (.png) and the final output file (.xlsx), are saved to the designated output folder.

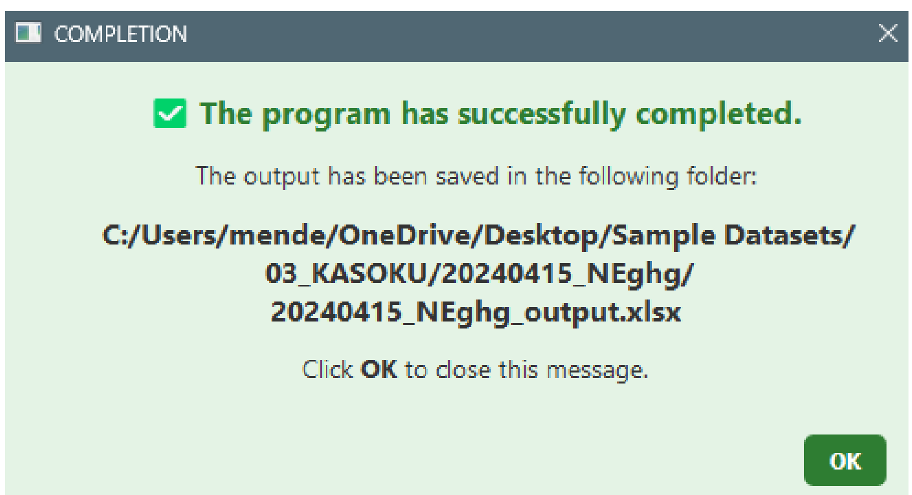


Figure 4.10. Kasoku Model Completion Window.

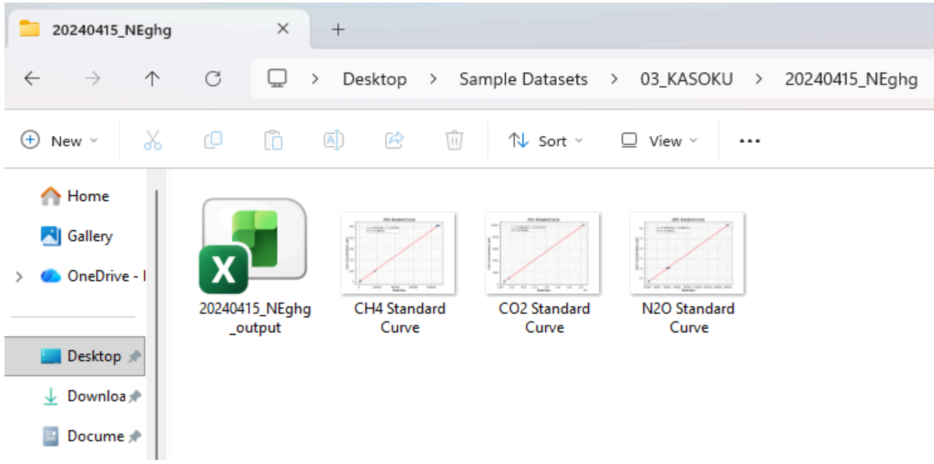
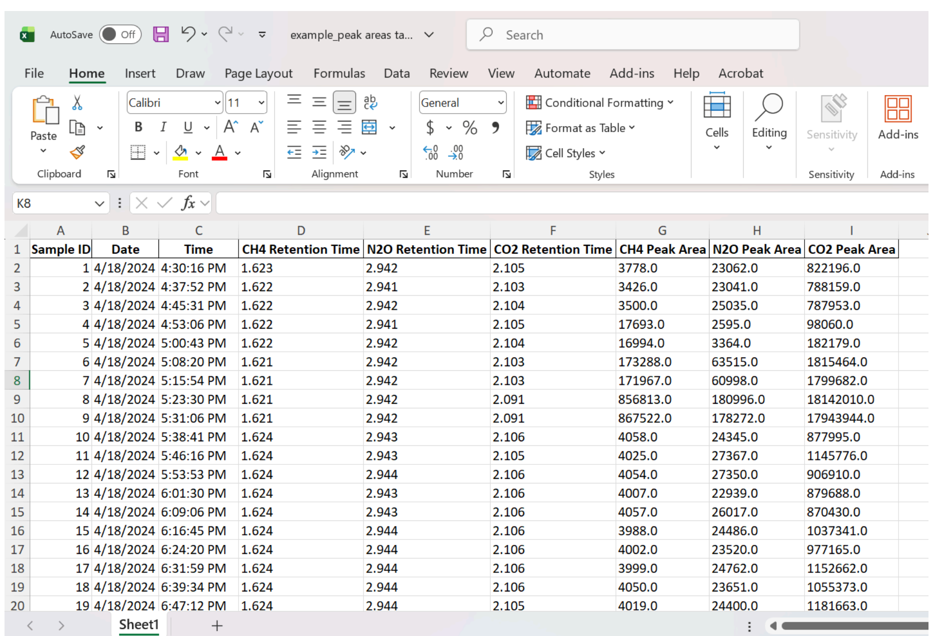


Figure 4.11. Output Excel File and Standard Curve Images

3. Input Specification

The Kasoku model requires the following inputs to be uploaded prior to analysis:

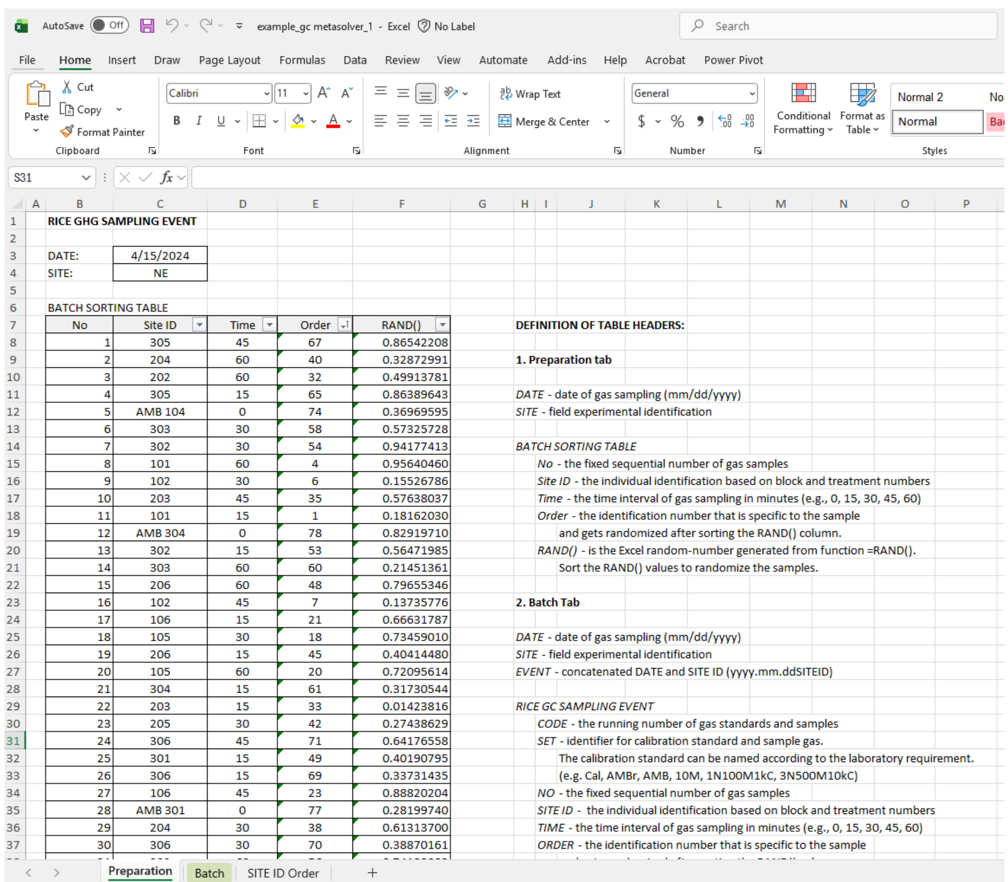
- *Peak Areas Table File (.xlsx)* - Excel format input file documenting each sample's unique identifier, analysis date, injection timestamp, retention times for CH_4, N_2O, and CO_2 gases, along with their corresponding peak area measurements.



Sample ID	Date	Time	CH4 Retention Time	N2O Retention Time	CO2 Retention Time	CH4 Peak Area	N2O Peak Area	CO2 Peak Area
1	4/18/2024	4:30:16 PM	1.623	2.942	2.105	3778.0	23062.0	822196.0
2	4/18/2024	4:37:52 PM	1.622	2.941	2.103	3426.0	23041.0	788159.0
3	4/18/2024	4:45:31 PM	1.622	2.942	2.104	3500.0	25035.0	787953.0
4	4/18/2024	4:53:06 PM	1.622	2.941	2.105	17693.0	2595.0	98060.0
5	4/18/2024	5:00:43 PM	1.622	2.942	2.104	16994.0	3364.0	182179.0
6	4/18/2024	5:08:20 PM	1.621	2.942	2.103	173288.0	63515.0	1815464.0
7	4/18/2024	5:15:54 PM	1.621	2.942	2.103	171967.0	60998.0	1799682.0
8	4/18/2024	5:23:30 PM	1.621	2.942	2.091	856813.0	180996.0	18142010.0
9	4/18/2024	5:31:06 PM	1.621	2.942	2.091	867522.0	178272.0	17943944.0
10	4/18/2024	5:38:41 PM	1.624	2.943	2.106	4058.0	24345.0	877995.0
11	4/18/2024	5:46:16 PM	1.624	2.943	2.105	4025.0	27367.0	1145776.0
12	4/18/2024	5:53:53 PM	1.624	2.944	2.106	4054.0	27350.0	906910.0
13	4/18/2024	6:01:30 PM	1.624	2.943	2.106	4007.0	22939.0	879688.0
14	4/18/2024	6:09:06 PM	1.624	2.943	2.106	4057.0	26017.0	870430.0
15	4/18/2024	6:16:45 PM	1.624	2.944	2.106	3988.0	24486.0	1037341.0
16	4/18/2024	6:24:20 PM	1.624	2.944	2.106	4002.0	23520.0	977165.0
17	4/18/2024	6:31:59 PM	1.624	2.944	2.106	3999.0	24762.0	1152662.0
18	4/18/2024	6:39:34 PM	1.624	2.944	2.106	4050.0	23651.0	1055373.0
19	4/18/2024	6:47:12 PM	1.624	2.944	2.105	4019.0	24400.0	1181663.0

Figure 4.12. GC Peak Area and Retention Time Summary in Excel format.

- *GC Metasolver (.xlsx)* - An Excel document that records how each batch was prepared prior to injection into the gas chromatography (GC) instrument. The file contains three worksheets namely *Preparation*, *Batch*, and *SITE ID Order*. Each worksheet provides specific details necessary for accurate and traceable sample preparation.
    - *Preparation worksheet* - Used to randomize gas samples for each batch by applying the RAND function.
    - *Batch worksheet* - Summary of complete randomized sampling event including standard gases.
    - *SITE ID Order worksheet* - Describes the ambient (AMB) gases distribution within the experimental site.



RICE GHG SAMPLING EVENT

DATE: 4/15/2024
SITE: NE

BATCH SORTING TABLE

No	Site ID	Time	Order	RAND()
1	305	45	67	0.86542208
2	204	60	40	0.32872991
3	202	60	32	0.49913781
4	305	15	65	0.86389643
5	AMB 104	0	74	0.36969595
6	303	30	58	0.57325728
7	302	30	54	0.94177413
8	101	60	4	0.95640460
9	102	30	6	0.15526786
10	203	45	35	0.57638037
11	101	15	1	0.18162030
12	AMB 304	0	78	0.82919710
13	302	15	53	0.56471985
14	303	60	60	0.21451361
15	206	60	48	0.79655346
16	102	45	7	0.13735776
17	106	15	21	0.66631787
18	105	30	18	0.73459010
19	206	15	45	0.40414480
20	105	60	20	0.72095614
21	304	15	61	0.31730544
22	203	15	33	0.01423816
23	205	30	42	0.27438629
24	306	45	71	0.64176558
25	301	15	49	0.40190795
26	306	15	69	0.33731435
27	106	45	23	0.88820204
28	AMB 301	0	77	0.28199740
29	204	30	38	0.61313700
30	306	30	70	0.38870161

DEFINITION OF TABLE HEADERS:

1. Preparation tab

DATE - date of gas sampling (mm/dd/yyyy)
SITE - field experimental identification

BATCH SORTING TABLE
No - the fixed sequential number of gas samples
Site ID - the individual identification based on block and treatment numbers
Time - the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60)
Order - the identification number that is specific to the sample and gets randomized after sorting the RAND() column.
RAND() - is the Excel random-number generated from function =RAND(). Sort the RAND() values to randomize the samples.

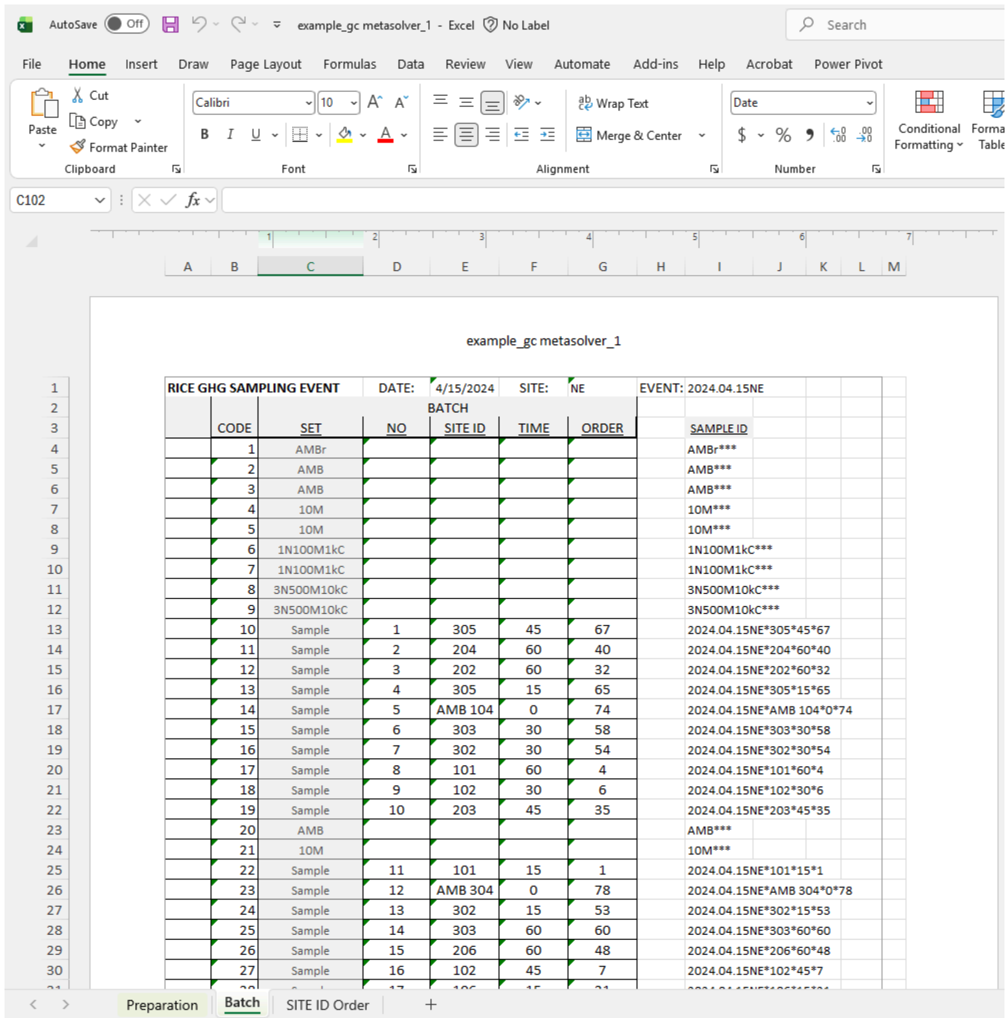
2. Batch Tab

DATE - date of gas sampling (mm/dd/yyyy)
SITE - field experimental identification
EVENT - concatenated DATE and SITE ID (yyyy.mm.ddSITEID)

RICE GC SAMPLING EVENT
CODE - the running number of gas standards and samples
SET - identifier for calibration standard and sample gas. The calibration standard can be named according to the laboratory requirement. (e.g. Cal, AMBr, AMB, 10M, 1N100M1kC, 3N500M10kC)
NO - the fixed sequential number of gas samples
SITE ID - the individual identification based on block and treatment numbers
TIME - the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60)
ORDER - the identification number that is specific to the sample

Preparation | Batch | SITE ID Order

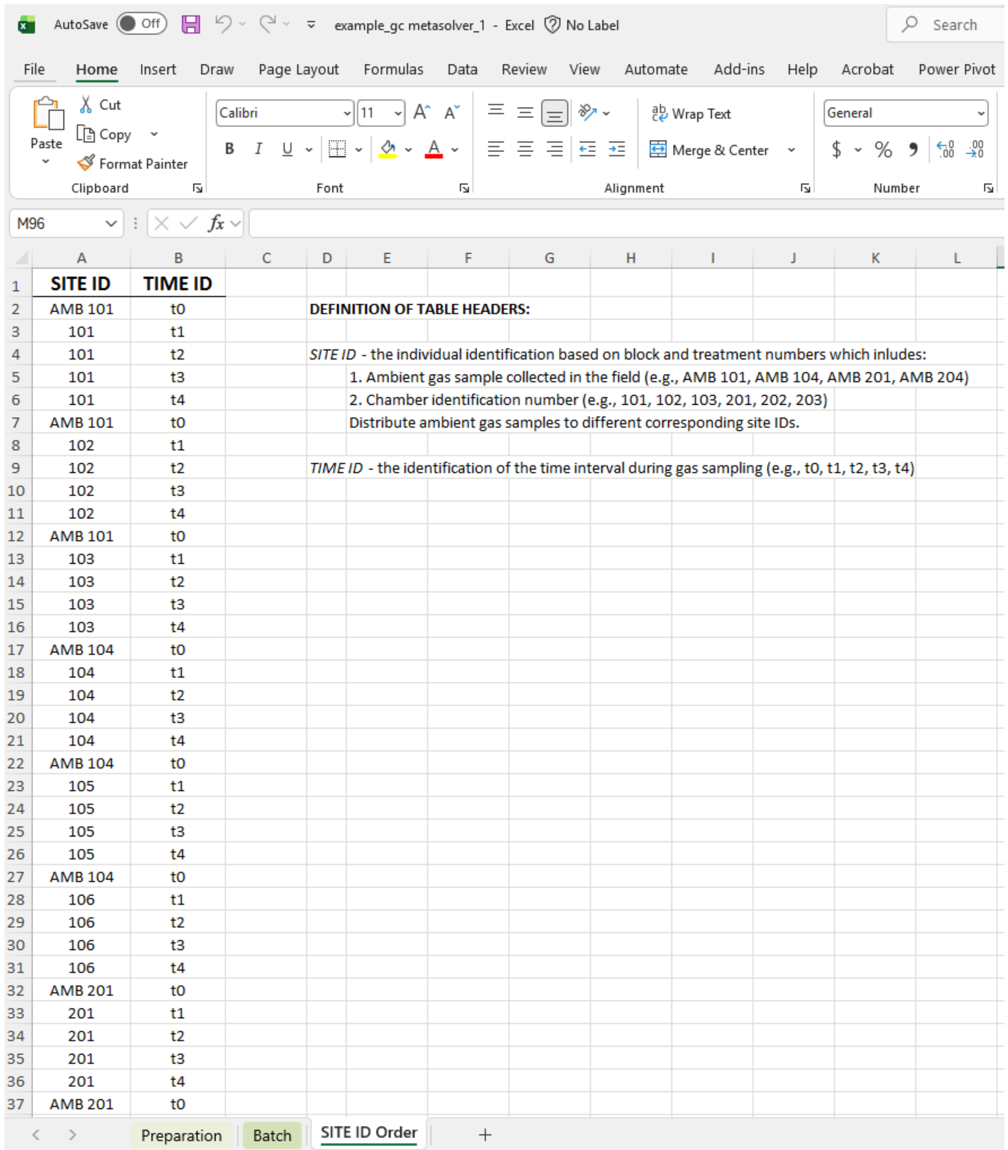
Figure 4.13. Preparation Worksheet in GC Metasolver.



example_gc metasolver_1

RICE GHG SAMPLING EVENT		DATE:	4/15/2024	SITE:	NE	EVENT:	2024.04.15NE
			BATCH				
	CODE	SET	NO	SITE ID	TIME	ORDER	SAMPLE ID
	1	AMBr					AMBr***
	2	AMB					AMB***
	3	AMB					AMB***
	4	10M					10M***
	5	10M					10M***
	6	1N100M1kC					1N100M1kC***
	7	1N100M1kC					1N100M1kC***
	8	3N500M10kC					3N500M10kC***
	9	3N500M10kC					3N500M10kC***
	10	Sample	1	305	45	67	2024.04.15NE*305*45*67
	11	Sample	2	204	60	40	2024.04.15NE*204*60*40
	12	Sample	3	202	60	32	2024.04.15NE*202*60*32
	13	Sample	4	305	15	65	2024.04.15NE*305*15*65
	14	Sample	5	AMB 104	0	74	2024.04.15NE*AMB 104*0*74
	15	Sample	6	303	30	58	2024.04.15NE*303*30*58
	16	Sample	7	302	30	54	2024.04.15NE*302*30*54
	17	Sample	8	101	60	4	2024.04.15NE*101*60*4
	18	Sample	9	102	30	6	2024.04.15NE*102*30*6
	19	Sample	10	203	45	35	2024.04.15NE*203*45*35
	20	AMB					AMB***
	21	10M					10M***
	22	Sample	11	101	15	1	2024.04.15NE*101*15*1
	23	Sample	12	AMB 304	0	78	2024.04.15NE*AMB 304*0*78
	24	Sample	13	302	15	53	2024.04.15NE*302*15*53
	25	Sample	14	303	60	60	2024.04.15NE*303*60*60
	26	Sample	15	206	60	48	2024.04.15NE*206*60*48
	27	Sample	16	102	45	7	2024.04.15NE*102*45*7

Figure 4.14. Example of Batch Worksheet in GC Metasolver.



SITE ID	TIME ID
AMB 101	t0
101	t1
101	t2
101	t3
101	t4
AMB 101	t0
102	t1
102	t2
102	t3
102	t4
AMB 101	t0
103	t1
103	t2
103	t3
103	t4
AMB 104	t0
104	t1
104	t2
104	t3
104	t4
AMB 104	t0
105	t1
105	t2
105	t3
105	t4
AMB 104	t0
106	t1
106	t2
106	t3
106	t4
AMB 201	t0
201	t1
201	t2
201	t3
201	t4
AMB 201	t0

DEFINITION OF TABLE HEADERS:

SITE ID - the individual identification based on block and treatment numbers which inludes:
1. Ambient gas sample collected in the field (e.g., AMB 101, AMB 104, AMB 201, AMB 204)
2. Chamber identification number (e.g., 101, 102, 103, 201, 202, 203)
Distribute ambient gas samples to different corresponding site IDs.

TIME ID - the identification of the time interval during gas sampling (e.g., t0, t1, t2, t3, t4)

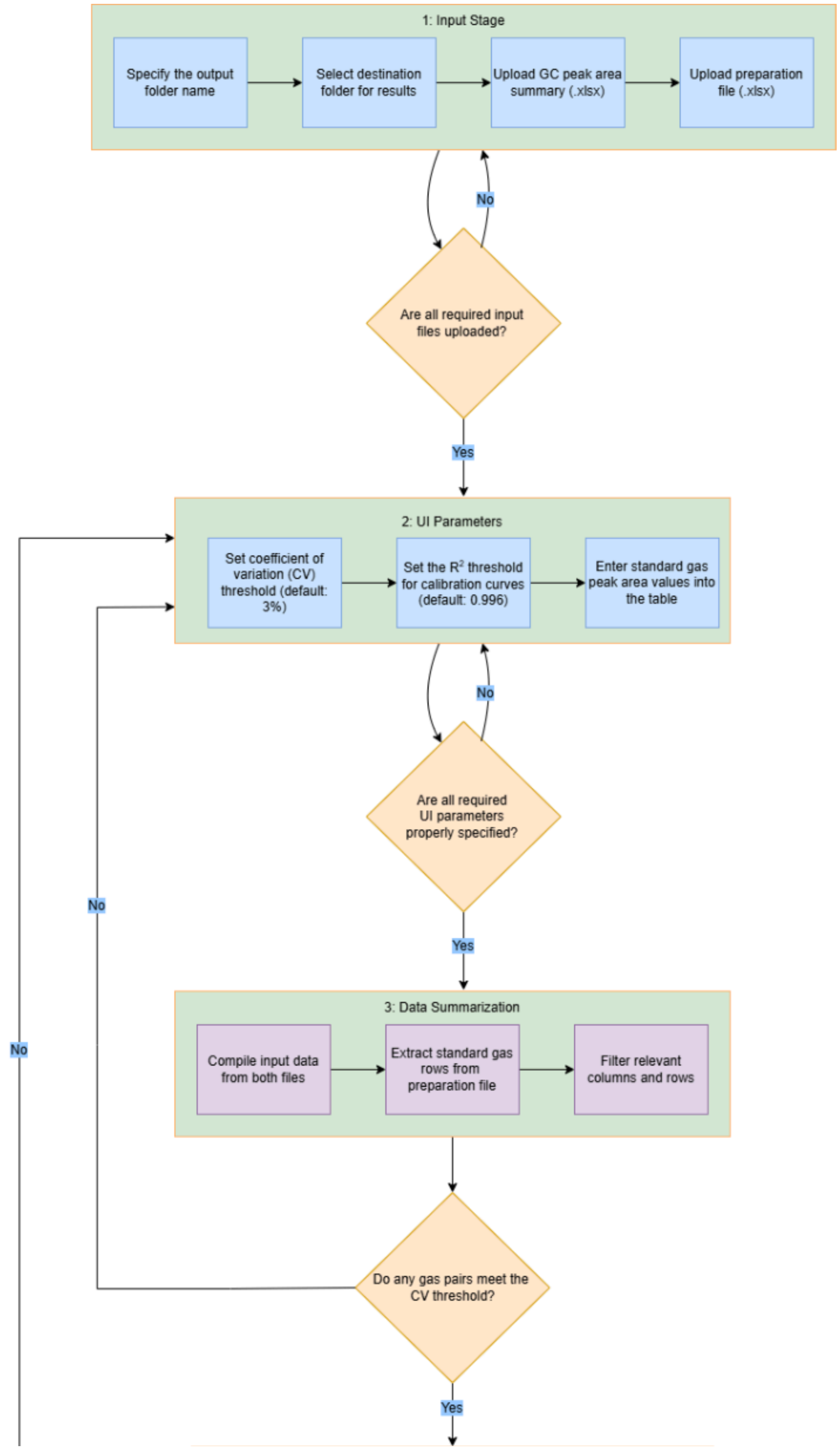
Figure 4.15. Example of SITE ID Order Worksheet in GC Metasolver.

4. Tips to Optimal Procedure

- Maintain the original headers of all example input files including the formatting and capitalization exactly as provided.
- Manually confirm that the number of samples in the Peaks Table File matches the number of samples in the Preparation File. The module does not enforce this check automatically and will continue processing even if the Peaks Table File contains fewer samples than the Preparation file. Mismatched sample counts may lead to incomplete calculations or missing outputs for specific gases.

- Maintain a site ID reference table and apply data validation rules in Excel to prevent mismatches during entry or copy-paste operations.
- To easily distinguish the GC summary from the preparation file, users may choose to name the files as follows:
  - date_SITEIDgc as the GC summary file name (e.g., 20250610_GF1gc, 20260105_NEgc)
  - date_SITEIDprep as the preparation file name (e.g., 20250610_GF1prep, 20260105_NEprep)
- For consistency, users may opt to label the Kasoku output folder using the format date_SITEIDghg (e.g., 20250610_GF1ghg, 20260105_NEghg).

5. Model Processing Flow



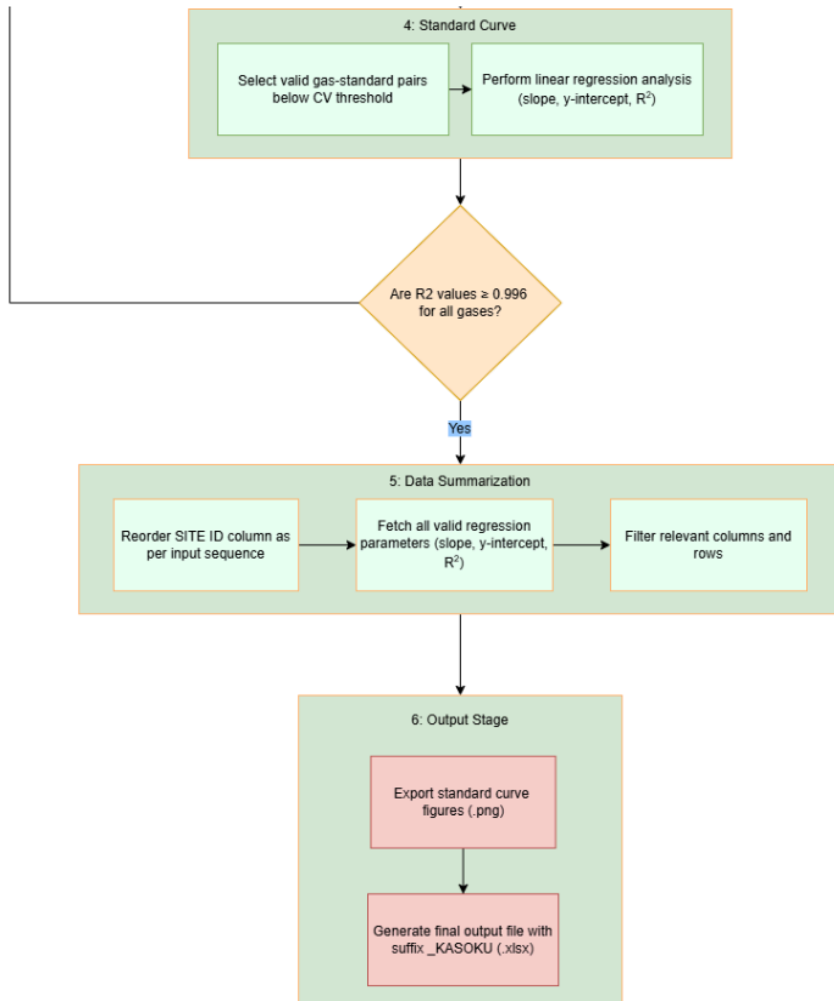


Figure 4.16. Model processing flow for DASIG-KASOKU Module.

6. Quality Assurance / Quality Control (QA/QC)

The Kasoku Model implements system checks to ensure accurate, precise and consistent trace-gas calculation from external standard curves. The components of QA/QC are:

- *Input Files Verification* - All required files (*GC Peak Area Summary and Preparation File*) are verified if uploaded to prevent incomplete or mismatched datasets from entering the pipeline.
- *UI Parameter Specification* - The user is required to define thresholds for CV (default: 3%) and R^2 values for calibration curves (default: 0.996 for all gas standards). These thresholds act as a filter to exclude noisy or imprecise data during the regression analysis.

- *Coefficient of Variation (CV) Filtering* - Prior to regression analysis, Kasoku model identifies gas-standard pairs that meet the defined CV threshold, where in CV is calculated as:

$$CV = \frac{Standard\ Deviation}{Mean} \ x\ 100$$

  Only datasets exhibiting acceptable precision, defined as value equal or below the specified CV threshold, advances to regression analysis. If the CV criterion is not met, the system will not generate a calibration curve. The CV threshold may be modified in the *CV Limit Input* field to reflect the user's required precision level.
- *Calibration Modeling* - Performs linear regression for each valid gas-standard pair. The output of this component are slope, y-intercept and R^2. This step ensures that the standard curve has strong linearity as confirmed by the user-defined R^2 value. If not met, the process loops back to refine threshold levels.
- *Data Summarization* - Reorders and aligns SITE ID and regression parameters for traceability. It filters the final dataset to include only valid regression outputs.
- *Final Quality Review* - Generates standard curve figures (.png) for visual inspection. The final result file (_KASOKU.xlsx) reports validated concentrations. The output stage ensures all outputs reflect only high-quality, threshold-compliant gas concentrations.

7. Output InterpretatioN

The Kasoku Model produces the following outputs:

- *Calibration Plot* - Illustrates the linear relationship between peak area and gas concentration (ppm) based on gas standard measurements. The red regression line follows the equation $y = mx + b$, with a coefficient of determination (R^2).

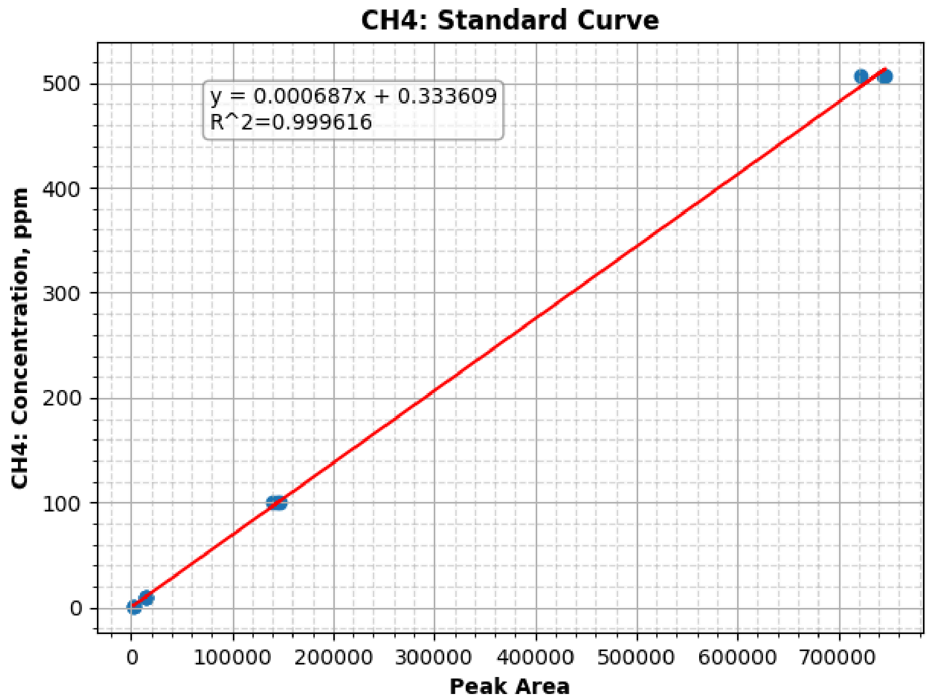
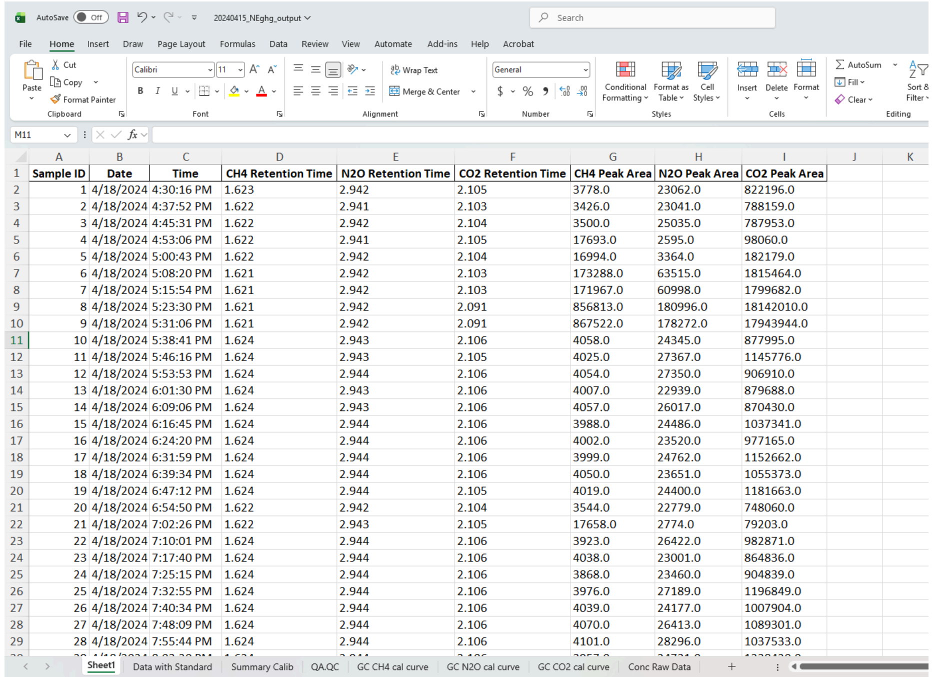


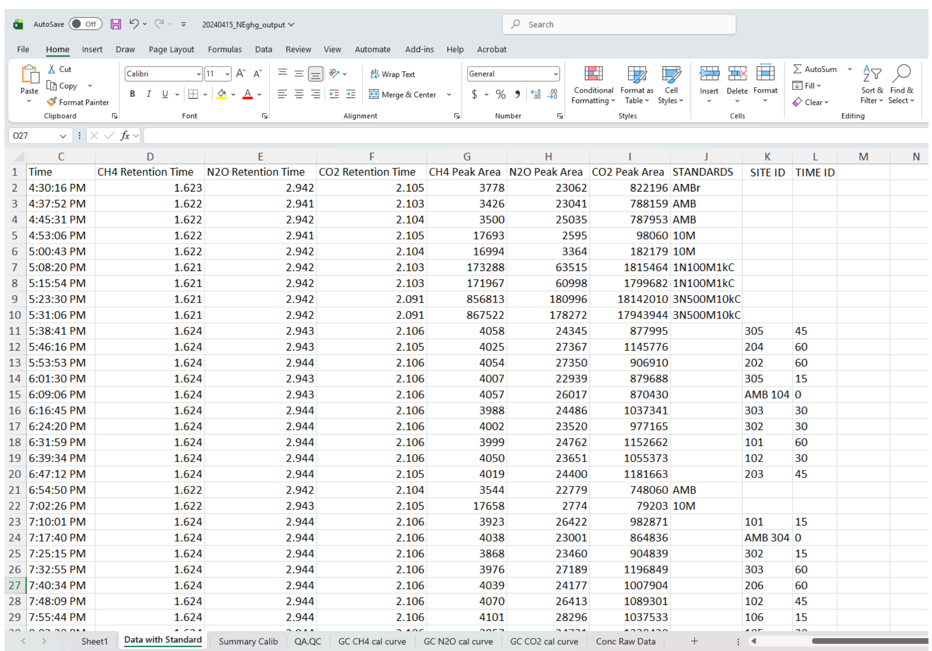
Figure 4.17. Calibration Curve for the Standard CH_4 Gas.

- *Kasoku Output* - An Excel file which consists of 8 spreadsheets containing the following information:
    - *Sheet 1* - Peak areas table file documenting each sample's unique identifier, analysis date, injection timestamp, retention times for CH_4, N_2O, and CO_2 gases, along with their corresponding peak area measurements.
    - *Data with Standard* - Serves as a filtered and annotated version of raw GC data integrating retention times for trace gas identification, peak areas for quantification, standard reference for calibration and quality assurance/quality control (QA/QC), site and time IDs for mapping concentrations across location and time intervals.



	Sample ID	Date	Time	CH4 Retention Time	N2O Retention Time	CO2 Retention Time	CH4 Peak Area	N2O Peak Area	CO2 Peak Area
2	1	4/18/2024	4:30:16 PM	1.623	2.942	2.105	3778.0	23062.0	822196.0
3	2	4/18/2024	4:37:52 PM	1.622	2.941	2.103	3426.0	23041.0	788159.0
4	3	4/18/2024	4:45:31 PM	1.622	2.942	2.104	3500.0	25035.0	787953.0
5	4	4/18/2024	4:53:06 PM	1.622	2.941	2.105	17693.0	2595.0	98060.0
6	5	4/18/2024	5:00:43 PM	1.622	2.942	2.104	16994.0	3364.0	182179.0
7	6	4/18/2024	5:08:20 PM	1.621	2.942	2.103	173288.0	63515.0	1815464.0
8	7	4/18/2024	5:15:54 PM	1.621	2.942	2.103	171967.0	60998.0	1799682.0
9	8	4/18/2024	5:23:30 PM	1.621	2.942	2.091	856813.0	180996.0	18142010.0
10	9	4/18/2024	5:31:06 PM	1.621	2.942	2.091	867522.0	178272.0	17943944.0
11	10	4/18/2024	5:38:41 PM	1.624	2.943	2.106	4058.0	24345.0	877995.0
12	11	4/18/2024	5:46:16 PM	1.624	2.943	2.105	4025.0	27367.0	1145776.0
13	12	4/18/2024	5:53:53 PM	1.624	2.944	2.106	4054.0	27350.0	906910.0
14	13	4/18/2024	6:01:30 PM	1.624	2.943	2.106	4007.0	22939.0	879688.0
15	14	4/18/2024	6:09:06 PM	1.624	2.943	2.106	4057.0	26017.0	870430.0
16	15	4/18/2024	6:16:45 PM	1.624	2.944	2.106	3988.0	24486.0	1037341.0
17	16	4/18/2024	6:24:20 PM	1.624	2.944	2.106	4002.0	23520.0	977165.0
18	17	4/18/2024	6:31:59 PM	1.624	2.944	2.106	3999.0	24762.0	1152662.0
19	18	4/18/2024	6:39:34 PM	1.624	2.944	2.106	4050.0	23651.0	1055373.0
20	19	4/18/2024	6:47:12 PM	1.624	2.944	2.105	4019.0	24400.0	1181663.0
21	20	4/18/2024	6:54:50 PM	1.622	2.942	2.104	3544.0	22779.0	748060.0
22	21	4/18/2024	7:02:26 PM	1.622	2.943	2.105	17658.0	2774.0	79203.0
23	22	4/18/2024	7:10:01 PM	1.624	2.944	2.106	3923.0	26422.0	982871.0
24	23	4/18/2024	7:17:40 PM	1.624	2.944	2.106	4038.0	23001.0	864836.0
25	24	4/18/2024	7:25:15 PM	1.624	2.944	2.106	3868.0	23460.0	904839.0
26	25	4/18/2024	7:32:55 PM	1.624	2.944	2.106	3976.0	27189.0	1196849.0
27	26	4/18/2024	7:40:34 PM	1.624	2.944	2.106	4039.0	24177.0	1007904.0
28	27	4/18/2024	7:48:09 PM	1.624	2.944	2.106	4070.0	26413.0	1089301.0
29	28	4/18/2024	7:55:44 PM	1.624	2.944	2.106	4101.0	28296.0	1037533.0

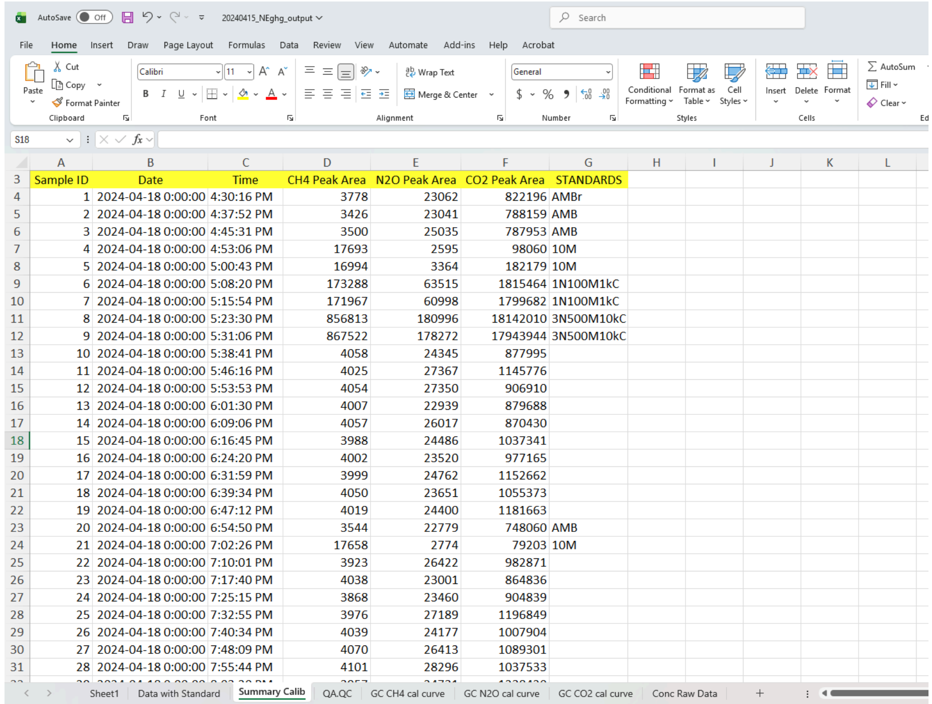
Figure 4.18. Peak Areas Table Repeated in Kasoku Output's Sheet 1



	Time	CH4 Retention Time	N2O Retention Time	CO2 Retention Time	CH4 Peak Area	N2O Peak Area	CO2 Peak Area	STANDARDS	SITE ID	TIME ID
2	4:30:16 PM	1.623	2.942	2.105	3778	23062	822196	AMBr		
3	4:37:52 PM	1.622	2.941	2.103	3426	23041	788159	AMB		
4	4:45:31 PM	1.622	2.942	2.104	3500	25035	787953	AMB		
5	4:53:06 PM	1.622	2.941	2.105	17693	2595	98060	10M		
6	5:00:43 PM	1.622	2.942	2.104	16994	3364	182179	10M		
7	5:08:20 PM	1.621	2.942	2.103	173288	63515	1815464	1N100M1kC		
8	5:15:54 PM	1.621	2.942	2.103	171967	60998	1799682	1N100M1kC		
9	5:23:30 PM	1.621	2.942	2.091	856813	180996	18142010	3N500M10kC		
10	5:31:06 PM	1.621	2.942	2.091	867522	178272	17943944	3N500M10kC		
11	5:38:41 PM	1.624	2.943	2.106	4058	24345	877995		305	45
12	5:46:16 PM	1.624	2.943	2.105	4025	27367	1145776		204	60
13	5:53:53 PM	1.624	2.944	2.106	4054	27350	906910		202	60
14	6:01:30 PM	1.624	2.943	2.106	4007	22939	879688		305	15
15	6:09:06 PM	1.624	2.943	2.106	4057	26017	870430		AMB 104	0
16	6:16:45 PM	1.624	2.944	2.106	3988	24486	1037341		303	30
17	6:24:20 PM	1.624	2.944	2.106	4002	23520	977165		302	30
18	6:31:59 PM	1.624	2.944	2.106	3999	24762	1152662		101	60
19	6:39:34 PM	1.624	2.944	2.106	4050	23651	1055373		102	30
20	6:47:12 PM	1.624	2.944	2.105	4019	24400	1181663		203	45
21	6:54:50 PM	1.622	2.942	2.104	3544	22779	748060	AMB		
22	7:02:26 PM	1.622	2.943	2.105	17658	2774	79203	10M		
23	7:10:01 PM	1.624	2.944	2.106	3923	26422	982871		101	15
24	7:17:40 PM	1.624	2.944	2.106	4038	23001	864836		AMB 304	0
25	7:25:15 PM	1.624	2.944	2.106	3868	23460	904839		302	15
26	7:32:55 PM	1.624	2.944	2.106	3976	27189	1196849		303	60
27	7:40:34 PM	1.624	2.944	2.106	4039	24177	1007904		206	60
28	7:48:09 PM	1.624	2.944	2.106	4070	26413	1089301		102	45
29	7:55:44 PM	1.624	2.944	2.106	4101	28296	1037533		106	15

Figure 4.19. GC Peak Areas Table File with Sample Description.

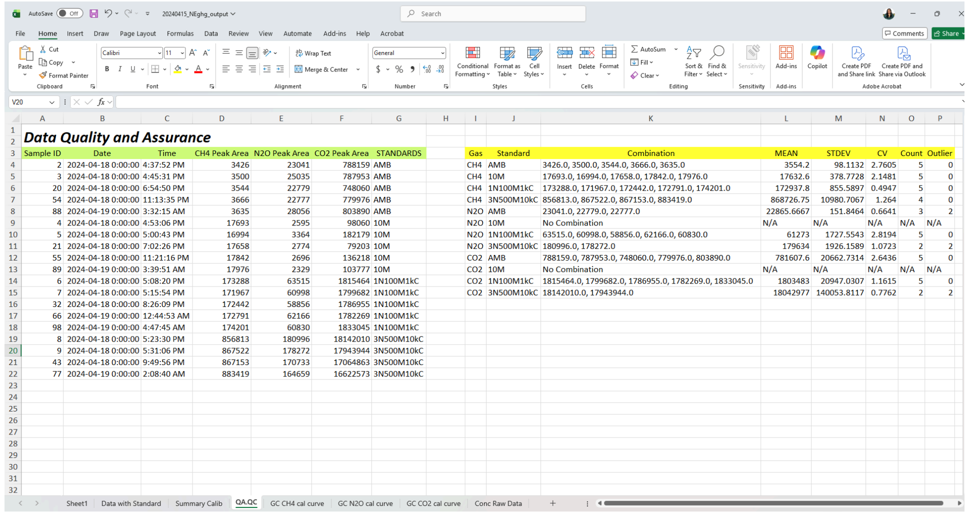
- *Summary Calib* - Presents a structured summary gas chromatography analysis results, with each row detailing a unique sample's metadata and corresponding peak area measurements for CH_4, N_2O, and CO_2 gases.



Sample ID	Date	Time	CH4 Peak Area	N2O Peak Area	CO2 Peak Area	STANDARDS
1	2024-04-18 0:00:00	4:30:16 PM	3778	23062	822196	AMBr
2	2024-04-18 0:00:00	4:37:52 PM	3426	23041	788159	AMB
3	2024-04-18 0:00:00	4:45:31 PM	3500	25035	787953	AMB
4	2024-04-18 0:00:00	4:53:06 PM	17693	2595	98060	10M
5	2024-04-18 0:00:00	5:00:43 PM	16994	3364	182179	10M
6	2024-04-18 0:00:00	5:08:20 PM	173288	63515	1815464	1N100M1kC
7	2024-04-18 0:00:00	5:15:54 PM	171967	60998	1799682	1N100M1kC
8	2024-04-18 0:00:00	5:23:30 PM	856813	180996	18142010	3N500M10kC
9	2024-04-18 0:00:00	5:31:06 PM	867522	178272	17943944	3N500M10kC
10	2024-04-18 0:00:00	5:38:41 PM	4058	24345	877995	
11	2024-04-18 0:00:00	5:46:16 PM	4025	27367	1145776	
12	2024-04-18 0:00:00	5:53:53 PM	4054	27350	906910	
13	2024-04-18 0:00:00	6:01:30 PM	4007	22939	879688	
14	2024-04-18 0:00:00	6:09:06 PM	4057	26017	870430	
15	2024-04-18 0:00:00	6:16:45 PM	3988	24486	1037341	
16	2024-04-18 0:00:00	6:24:20 PM	4002	23520	977165	
17	2024-04-18 0:00:00	6:31:59 PM	3999	24762	1152662	
18	2024-04-18 0:00:00	6:39:34 PM	4050	23651	1055373	
19	2024-04-18 0:00:00	6:47:12 PM	4019	24400	1181663	
20	2024-04-18 0:00:00	6:54:50 PM	3544	22779	748060	AMB
21	2024-04-18 0:00:00	7:02:26 PM	17658	2774	79203	10M
22	2024-04-18 0:00:00	7:10:01 PM	3923	26422	982871	
23	2024-04-18 0:00:00	7:17:40 PM	4038	23001	864836	
24	2024-04-18 0:00:00	7:25:15 PM	3868	23460	904839	
25	2024-04-18 0:00:00	7:32:55 PM	3976	27189	1196849	
26	2024-04-18 0:00:00	7:40:34 PM	4039	24177	1007904	
27	2024-04-18 0:00:00	7:48:09 PM	4070	26413	1089301	
28	2024-04-18 0:00:00	7:55:44 PM	4101	28296	1037533	

Figure 4.20. Summary Description of the Gas Sample.

- *QA.QC* - Summarizes the external gas standards used for trace-gas quantification through calibration curve. This spreadsheet is designed to assess the precision, consistency, and overall reliability of gas chromatography measurement across multiple calibration standards. The QA/QC table reports the target analyte, the calibration standard used, the combination of peak areas used for analysis, and the resulting statistical metrics, including mean, standard deviation, coefficient of variation, sample count and identified outlier.



Data Quality and Assurance

Sample ID	Date	Time	CH4 Peak Area	N2O Peak Area	CO2 Peak Area	STANDARDS
2	2024-04-18 0:00:00	4:37:52 PM	3426	23041	788159	AMB
3	2024-04-18 0:00:00	4:45:31 PM	3500	25035	787953	AMB
20	2024-04-18 0:00:00	6:54:50 PM	3544	22779	748060	AMB
54	2024-04-18 0:00:00	11:13:35 PM	3666	22777	779976	AMB
88	2024-04-19 0:00:00	3:32:15 AM	3635	28056	803890	AMB
4	2024-04-18 0:00:00	4:53:06 PM	17693	2595	98060	10M
5	2024-04-18 0:00:00	5:00:43 PM	16994	3364	182179	10M
21	2024-04-18 0:00:00	7:02:26 PM	17658	2774	79203	10M
55	2024-04-18 0:00:00	11:21:16 PM	17842	2696	136218	10M
89	2024-04-19 0:00:00	3:39:51 AM	17976	2329	103777	10M
6	2024-04-18 0:00:00	5:08:20 PM	173288	63515	1815464	1N100M1kC
7	2024-04-18 0:00:00	5:15:54 PM	171967	60998	1799682	1N100M1kC
32	2024-04-18 0:00:00	8:26:09 PM	172442	58856	1786955	1N100M1kC
66	2024-04-19 0:00:00	12:44:53 AM	172791	62166	1782269	1N100M1kC
98	2024-04-19 0:00:00	4:47:45 AM	174201	60830	1833045	1N100M1kC
8	2024-04-18 0:00:00	5:23:30 PM	856813	180996	18142010	3N500M10kC
9	2024-04-18 0:00:00	5:31:06 PM	867522	178272	17943944	3N500M10kC
43	2024-04-18 0:00:00	9:49:56 PM	867153	170733	17064863	3N500M10kC
77	2024-04-19 0:00:00	2:08:40 AM	883419	164659	16622573	3N500M10kC

Gas	Standard	Combination	MEAN	STDEV	CV	Count	Outlier
CH4	AMB	3426.0, 3500.0, 3544.0, 3666.0, 3635.0	3554.2	98.1132	2.7605	5	0
CH4	10M	17693.0, 16994.0, 17658.0, 17842.0, 17976.0	17632.6	378.7728	2.1481	5	0
CH4	1N100M1kC	173288.0, 171967.0, 172442.0, 172791.0, 174201.0	172937.8	855.5897	0.4947	5	0
CH4	3N500M10kC	856813.0, 867522.0, 867153.0, 883419.0	868726.75	10980.7067	1.264	4	0
N2O	AMB	23041.0, 22779.0, 22777.0	22865.6667	151.8464	0.6641	3	2
N2O	10M	No Combination	N/A	N/A	N/A	N/A	N/A
N2O	1N100M1kC	63515.0, 60998.0, 58856.0, 62166.0, 60830.0	61273	1727.5543	2.8194	5	0
N2O	3N500M10kC	180996.0, 178272.0	179634	1926.1589	1.0723	2	2
CO2	AMB	788159.0, 787953.0, 748060.0, 779976.0, 803890.0	781607.6	20662.7314	2.6436	5	0
CO2	10M	No Combination	N/A	N/A	N/A	N/A	N/A
CO2	1N100M1kC	1815464.0, 1799682.0, 1786955.0, 1782269.0, 1833045.0	1803483	20947.0307	1.1615	5	0
CO2	3N500M10kC	18142010.0, 17943944.0	18042977	140053.8117	0.7762	2	2

Figure 4.21. Data Quality and Assurance Report for the GC Analysis.

- *GC CH_4/N_2O/CO_2 cal curve* - Presents a detailed calibration workflow for quantifying methane (CH_4), nitrous oxide (N_2O), carbon dioxide (CO_2) concentrations using a GC instrument.

  The worksheets combine raw data, regression analysis, and concentration calculations to validate the accuracy and linearity of the method. The gas standards table lists known gas concentration and peak area used to build the curve. The output includes a graph explaining how standard gas concentration correlates with peak area. The regression equation and R^2 values were also presented together with the standard curve graph.

  The regression analysis table presents comparative regression output across multiple calibration ranges. It reports the slope, y-intercept, R^2, and number observations, allowing evaluation of calibration performance across distinct concentration intervals.

  Each worksheet also includes a table of calculated standard-gas concentrations derived from peak areas using multiple regression models, ranging from full calibration dataset (*All Data*) to subsets restricted to three (*e.g., To 100.3 ppm for CH_4*) or two (*e.g., To 1.01 ppm for N_2O, To 992.3 ppm for CO_2*) concentration levels. This section is used to assess the consistency of calculated concentrations relative to the concentration range of the samples. The Kasoku model then identifies the most appropriate values for reporting and for constructing the final calculation curve; these selected values are shown in the table as *FINAL PPM*.

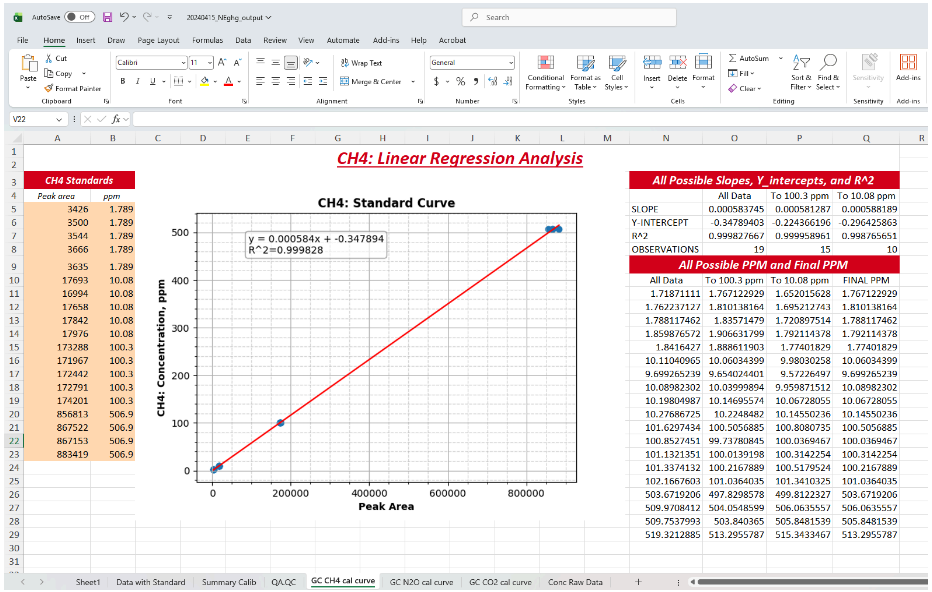


Figure 4.22. Linear Regression Analysis of the Standard CH_4 Gas.

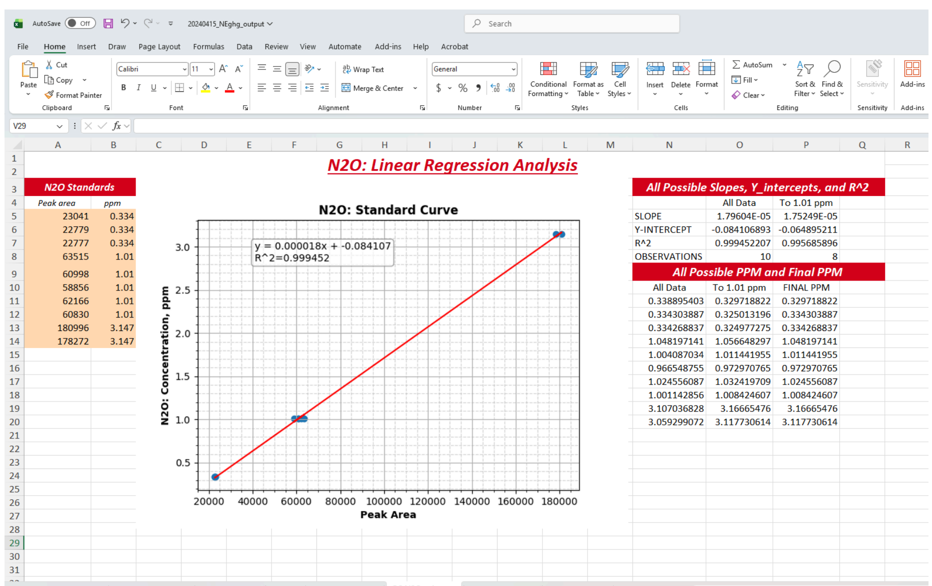


Figure 4.23. Linear Regression Analysis of the Standard N_2O Gas.

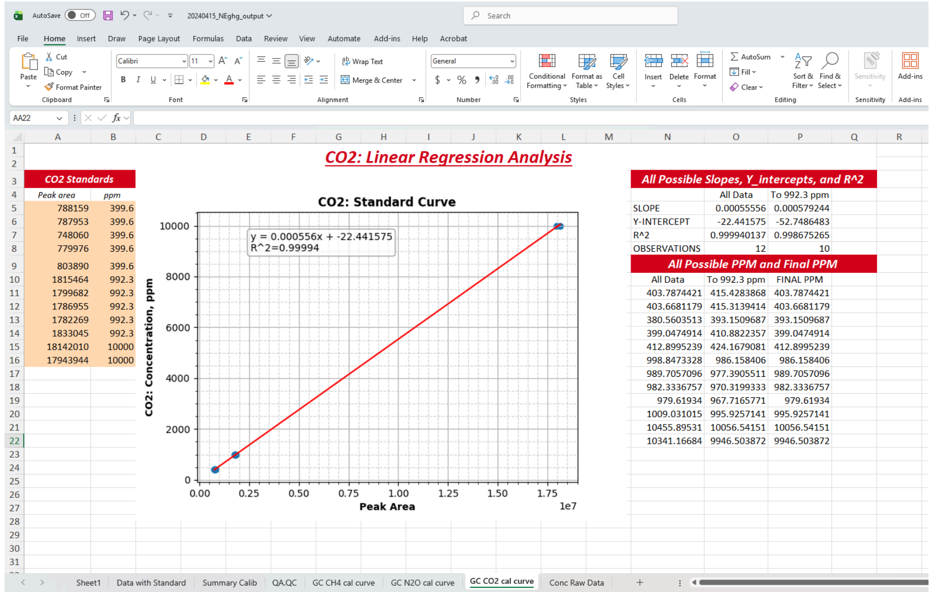


Figure 4.24. Linear Regression Analysis of the Standard CO_2 Gas.

- *Conc Raw Data*- Presents a comprehensive summary of gas concentration for CH_4, N_2O and CO_2 using the previously selected calibration curves. It combines calibration parameters SITE ID-specific peak area data to compute final concentrations.

  The left section of the worksheet summarizes multiple regression models used to convert the peak area into gas concentration. It compiles calibration parameters including slope, y-intercept, R^2, and number of observations, across different concentration ranges and gas standards (CH_4, N_2O and CO_2). High R^2 values indicate strong linearity and reliable performance of the calibration curve.

  In the right or main section of the worksheet the selected calibration curve parameters are applied to the actual sample data, where in:

  - *SITE ID and TIME ID* identify each sample.
  - *PEAK AREA* refers to the raw detector response.
  - *SLOPE* and *Y-INTERCEPT* values are taken from the calibration model that demonstrates the highest accuracy and precision.
  - *CONCENTRATION* is calculated using the linear regression formula:

$$Concentration\ (ppm) = (Peak\ Area\ x\ Slope) + Y - intercept$$

Each trace gas has its own columns and the final concentration values are highlighted in *RED* for clarity.

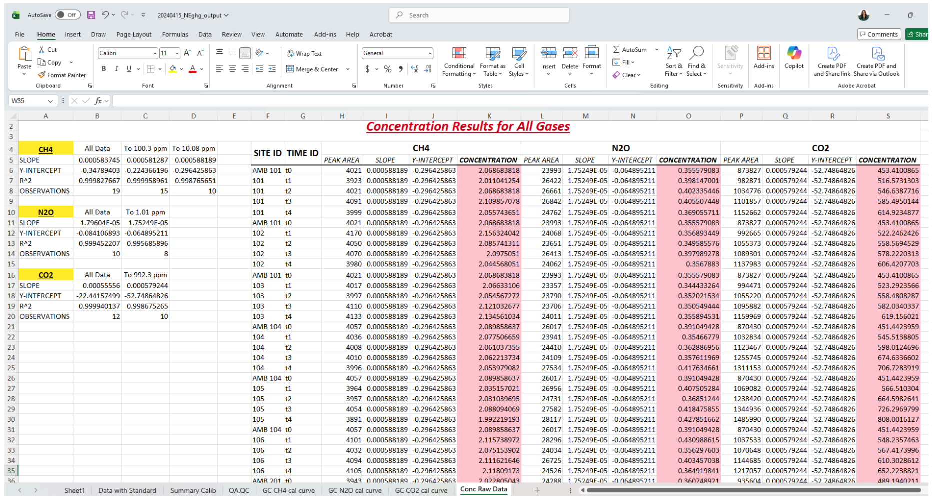


Figure 4.25. Calculated Concentration for All Trace Gases.

8. Troubleshooting

Issue: File Assignment Error

The GC Peak Summary and Preparation File were uploaded to the incorrect input fields. When the user uploaded the input files in reversed order, it will result to a file-type mismatch because the uploaded Peaks Table file (e.g., example_gc_summary_1.xlsx) does not contain all the columns that the software expects for proper parsing and analysis. Missing columns are:

- Sample ID
- Date
- Time
- CH_4 Retention Time
- N_2O Retention Time
- CO_2 Retention Time
- CH_4 Peak Area
- N_2O Peak Area
- CO_2 Peak Area

Impact: Without these columns, the Kasoku Module cannot extract retention times or peak area target gases (CH_4, N_2O, and CO_2), nor can it associate them with sample metadata (SITE ID, date, and time). This halts the workflow before regression or quantification steps.

Resolution:

a. Load the Peak Areas Table into the Peaks Input field. This file must contain all required columns (Sample ID, Date, Time, Retention Times, and Peak Areas).
b. Load the Prep File into the Prep Input field. This file contains preparation and standard-related metadata.
c. Verify that column names in the Peak Table match the required format exactly with no missing fields, no extra spaces, and correct spelling.
d. Re-upload both files after correcting the assignments. Once the correct files are in the correct slots, the Kasoku Module will validate them and proceed normally.

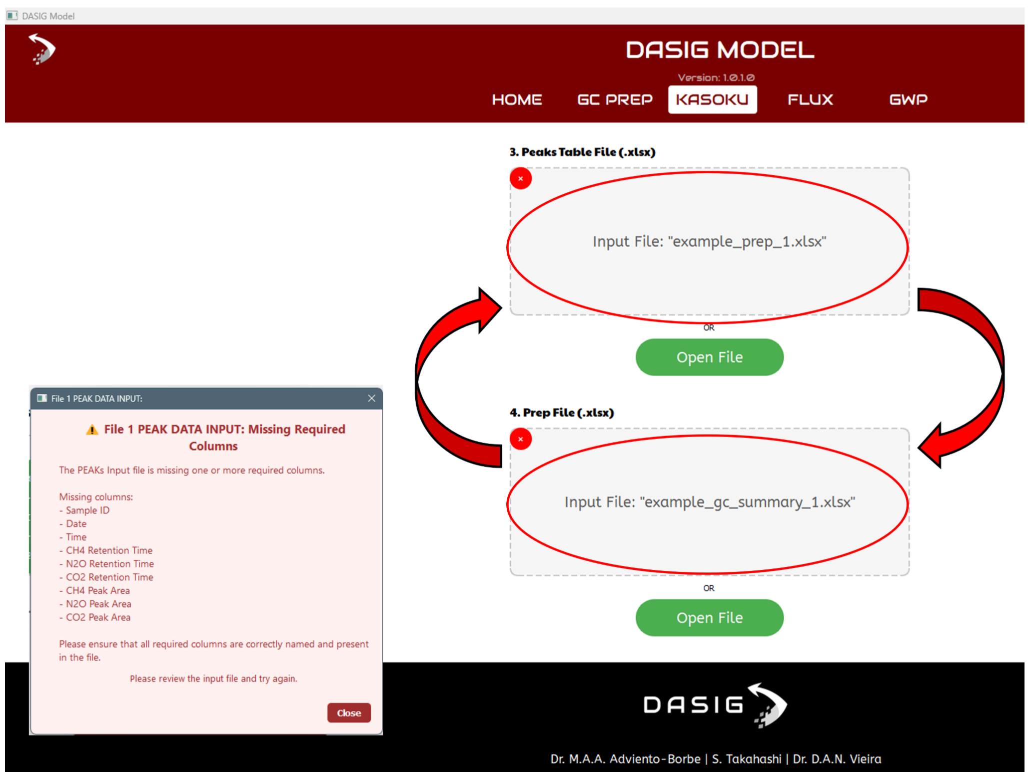


Figure 4.26. File Assignment Error.

Issue: Missing Retention Time and Peak Area Error

This error message from Kasoku Module indicated that regression analysis cannot proceed because the program was unable to compute a valid CV for a specific gas. The module could not identify a valid set of peak area values that meet the criteria for calculating CV for a specific gas. This typically occurs when:

- Peak Area values are missing, zero, or non-numeric in one or more rows.
- Standard pairs or replicates required for CV computation are incomplete or improperly formatted
- Data fails QA/QC thresholds, such as excessive variability or missing retention times.

Impact: The CV cannot be calculated for the gas with missing Retention Time and Peak Area values. In the absence of a valid CV, the system will terminate regression analysis for that specific gas, and a calibration curve will not be generated.

Resolution:

a. Review the Peak Area column in the Peaks Tables File for missing or invalid entries.
b. Confirm that all required rows contain numeric values and that replicate standards are properly grouped.
c. Re-upload the corrected file and re-run the analysis.

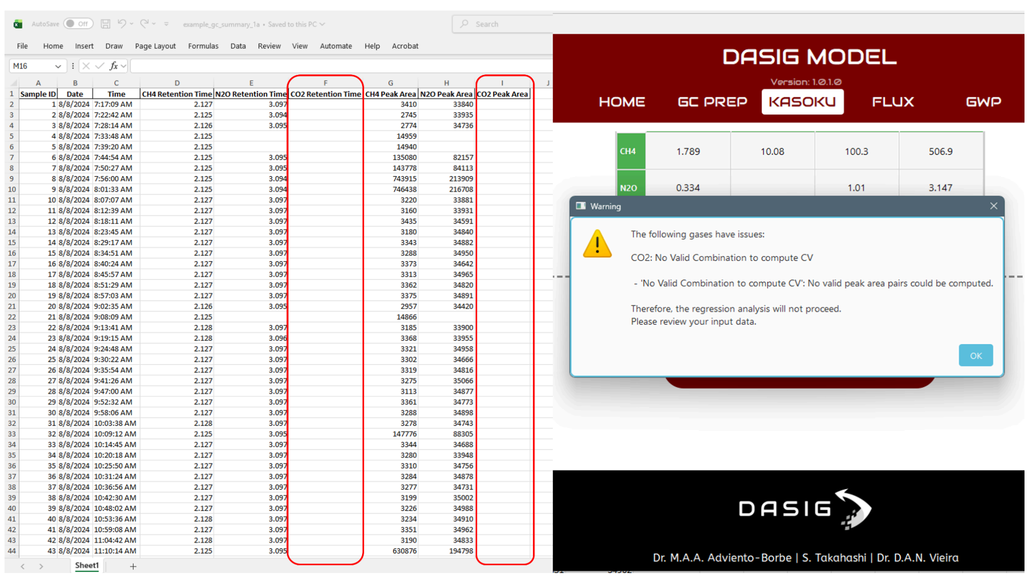


Figure 4.27. Missing Retention Time and Peak Area Error.

Issue: Column Header Error

This error is triggered because the uploaded input file does not contain the required column headers in the expected format. The required column for the Peak Table File are as follows:

- Sample ID
- Date
- Time
- CH_4 Retention Time
- N_2O Retention Time
- CO_2 Retention Time
- CH_4 Peak Area
- N_2O Peak Area
- CO_2 Peak Area

Impact: Discrepancies in the column headers prevent the software from recognizing and parsing the data correctly. As a result, the program is unable to compute the CV for each gas, which is a prerequisite for initiating regression analysis. Without valid CV values, the system halts all curve-fitting procedures, and no calibration curves are produced. This interruption directly impacts downstream quantification and reporting, rendering the dataset unusable for concentration calculations until the input file is corrected.

Resolution:

a. Rename all column headers to match the required format exactly. For example:
    i. Use *Sample ID*, not *ID*.
    ii. Use *Time*, not *TIME*.
    iii. Use *CH_4 Retention Time*, not *CH_4 Retention Time*.
    iv. Use *N_2O Peak Area*, not *N_2O_PeakArea*.
    v. Use *CO_2 Peak Are*, not *CO_2 Peak*.
b. Ensure there are no extra spaces, typos, or formatting inconsistencies.
c. Save the corrected file in *.xlsx* format and re-upload.

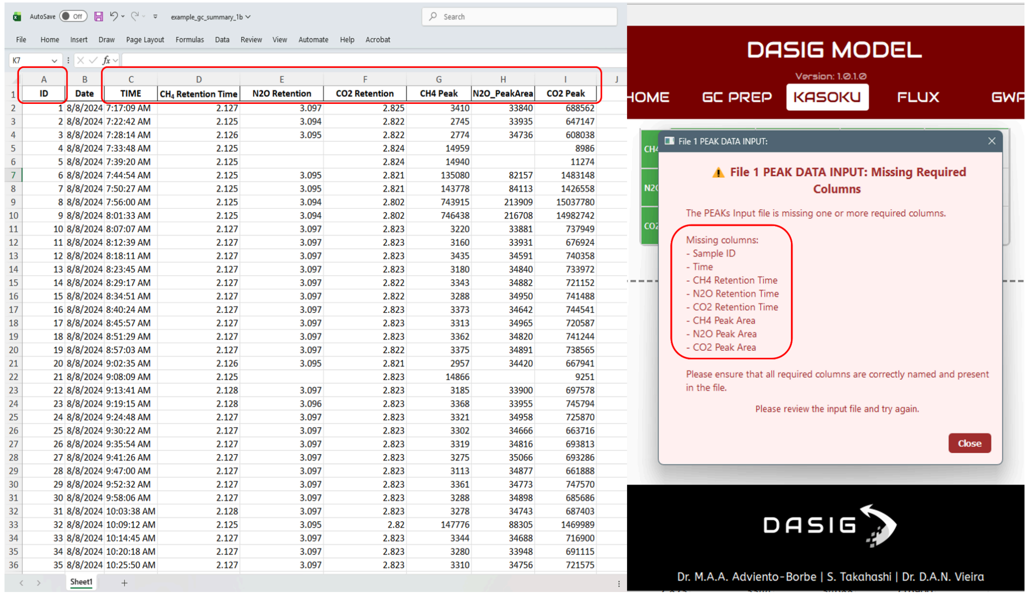


Figure 4.28. Incorrect Column Headers.

Issue: Output Folder Duplication

This error message indicated a folder name duplication conflict during output file generation. The user entered an output folder name (e.g., *Test*) that already exists in the designated working directory. The module is designed to prevent overwriting existing folders to preserve prior results and maintain data integrity.

Impact: To prevent accidental overwriting of existing results, the module immediately halts output generation when a duplicate folder is detected. No new files will be created or saved until the user provides a unique folder name.

Resolution:

a. Enter a new, unused folder name in the *Output Folder Name* field.
b. Confirm that the name does not already exist in the working directory path.
c. Click *OK* to close the warning and re-submit with the revised folder name.

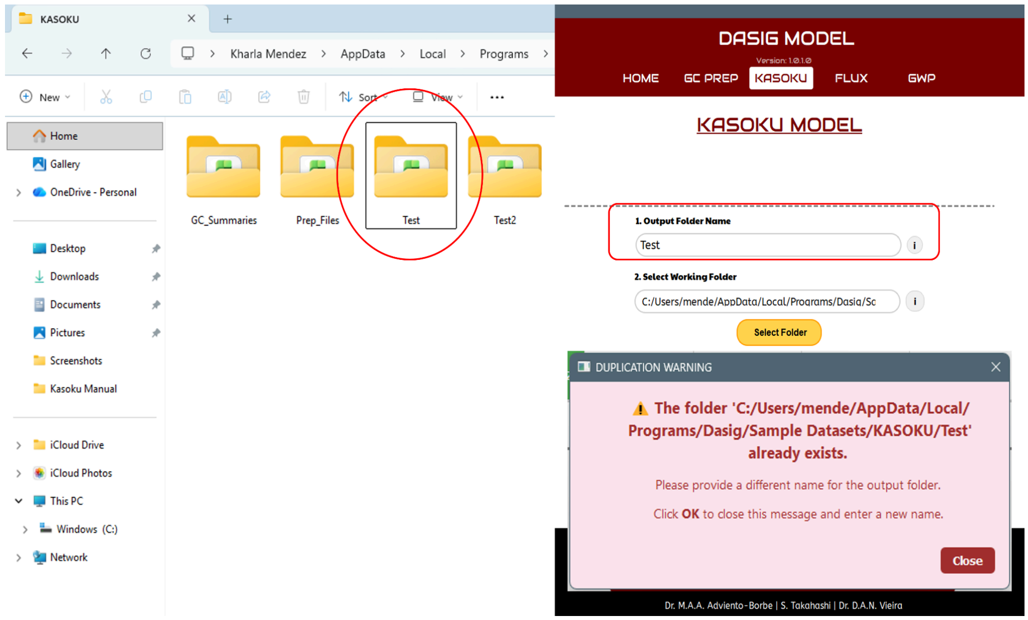


Figure 4.29. Output Folder Name Duplication Warning.

Issue: SITE ID Mismatch

This error is triggered when the SITE ID Order and Batch worksheets contain non-matching site identifiers, preventing proper alignment of sample metadata. The module performs a bidirectional check to ensure all site IDs are consistently represented across worksheets.

- In Figure …, the following site IDs appear in *SITE ID Order* but are missing from *Batch*: *102, 103, 105, 106, 202, 203, 206, 301, 305, 306, AMB_MN_1, AMB_MN_2, AMB_MN_3, AMB_MN_4, and AMB__MN_5*.
- The SITE IDs listed in the SITE ID Order worksheet differ from those used in the *Preparation* and *Batch* worksheets, resulting in a mismatch that prevents proper sample alignment during data validation (Figure …).

Impact: The module cannot proceed with sample alignment or gas concentration calculations with SITE ID mismatch. Missing site IDs may result in incomplete data processing, skipped samples, or invalid batch assignments. This error blocks execution until resolved.

Resolution:

a. Open the *Preparation File* and verify both sheets:
    i. *SITE ID Order* - contains the expected sequence of site IDs.
    ii. *Batch* - must include matching site IDs for each entry.
b. Confirm that the *SAMPLE ID* column in the *Batch* worksheet contains properly concatenated values for each entry. Specifically, ensure that the following fields are included and formatted consistently:
    i. *SET*
    ii. *DESCRIPTION*
    iii. *SITE ID*
    iv. *TIME*
    v. *ORDER*

   This concatenation must be applied to all samples and standards to maintain alignment across the dataset and enable accurate downstream processing.
c. Ensure column headers are correct in both sheets.
d. Check for common issues:
    i. Typos or extra spaces in site IDs (e.g., AMB_MN_1 vs AMB_1).
    ii. Missing rows or accidental deletions.
    iii. Incorrect sheet names and column headers.
e. Update site IDs to match across sheets.
f. Re-upload the corrected Preparation File to the Kasoku Module.

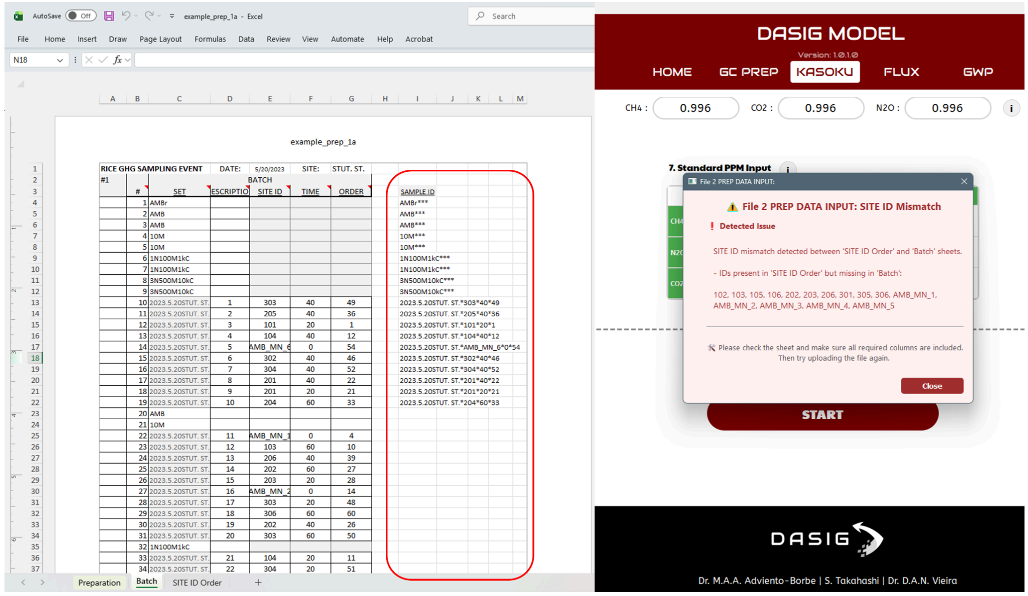


Figure 4.30. Site ID Mismatch Error Resulting from Incomplete SAMPLE ID Concatenation.

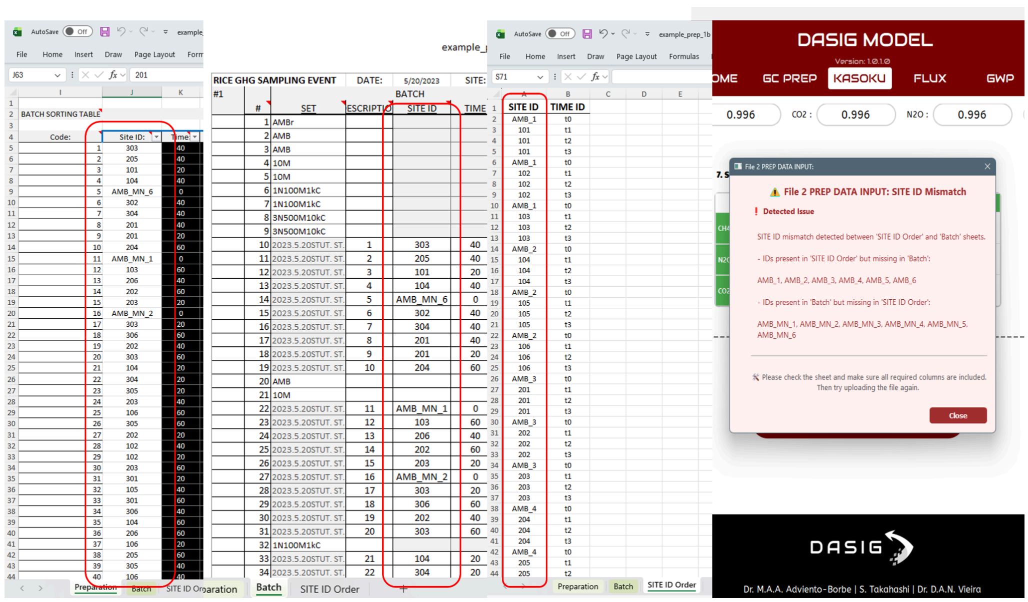


Figure 4.31. Site ID Mismatch Across Preparation File Sheet.

Issue: No Valid Combination to Compute CV

This error indicates that no valid combinations of peak areas were found, preventing the calculations of the CV and halting regression analysis. The module cannot identify a valid set of peak area values associated with standard entries. The error typically occurs when:

- Standard identifiers are missing or inconsistent in the Preparation File or Peak Areas Table.
- Peak area values are present but not properly grouped or matched to standards.
- Replicate standards are not detected, or combinations fail internal validation rules.

Impact: Without valid peak-area pairs, the software cannot evaluate precision or generate a calibration curve, so the regression step for the gas being quantified is skipped entirely. As a result, no slope, intercept, R^2, or QC metrics are produced, and any downstream calculations or summaries will be incomplete or omitted.

Resolution:

a. Review GC Metasolver and Peaks Table File to ensure the standard samples are correctly labeled and consistently formatted.
b. Confirm that the peak areas are present for all standard entries and that replicate groups are properly defined.
c. Re-upload corrected files and re-run the module.
d. Repeat GC analyses of the batch to obtain high quality data.

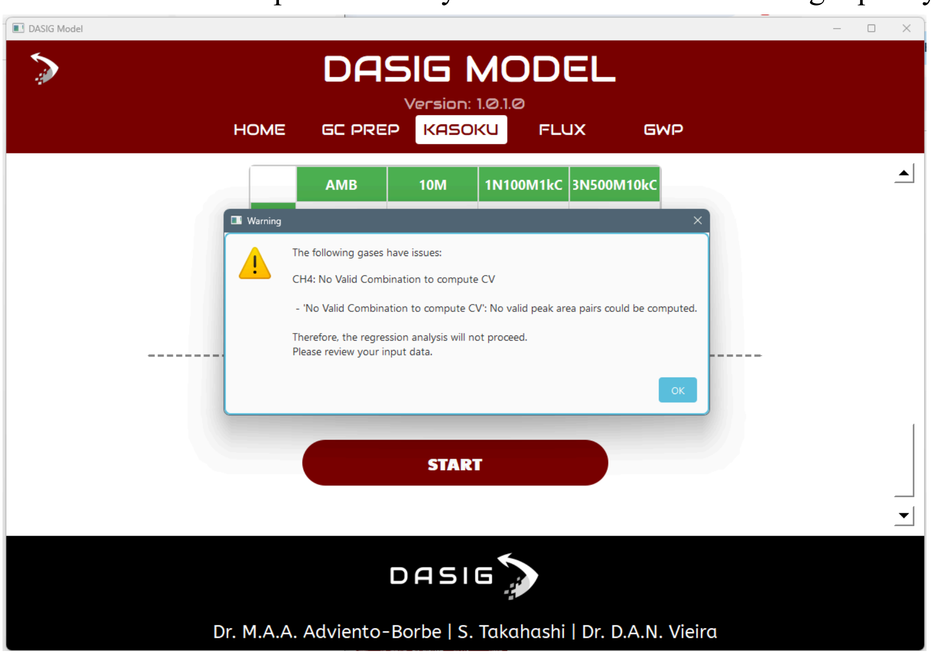


Figure 4.32. Standard Curve Failure Due to Invalid Peak Area Combination.

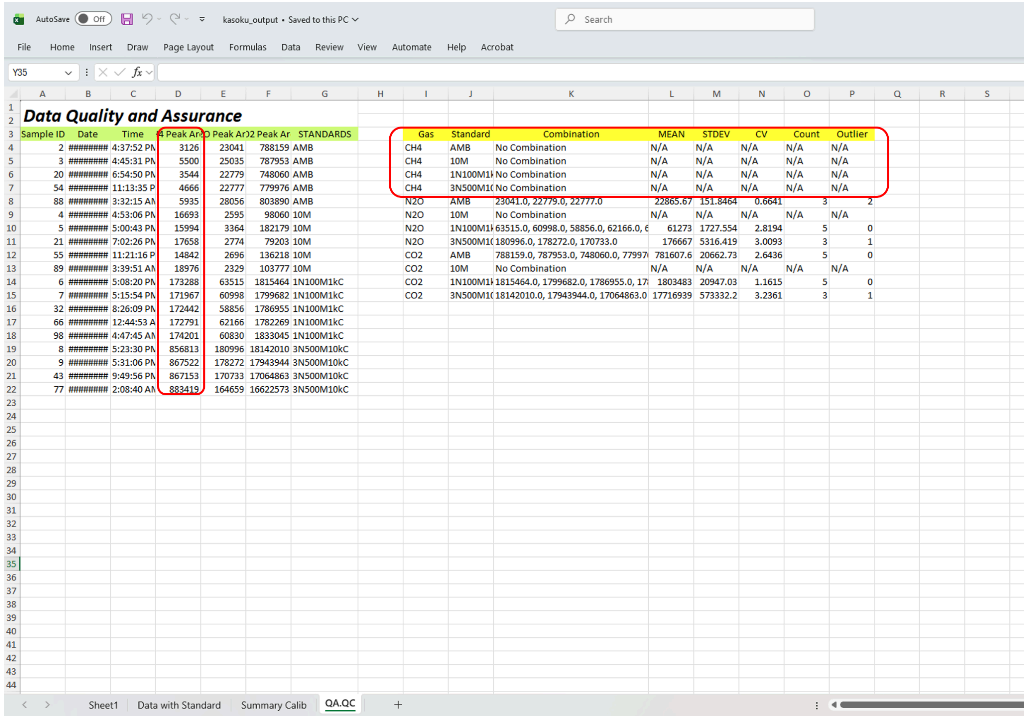


Figure 4.33. Summary of Peak Area Variability with CH_4 Marked as No Combination.

9. Glossary

Term	Definition
Batch (worksheet)	Summary of complete randomized sampling event including standard gases.
CH_4 Peak Area	Peak area for methane.
CH_4 Retention Time	Retention time for methane.
N_2O Peak Area	Peak area for nitrous oxide
N_2O Retention Time	Retention time for nitrous oxide.
CO_2 Peak Area	Peak area for carbon dioxide.
CO_2 Retention Time	Retention time for carbon dioxide.
Coefficient of Variance (CV)	Statistical measure that expresses the amount of variability in each standard gas relative to its mean.

Coefficient of Determination (R^2)	Indicates the linearity and reliability for quantifying standard gas from peak area data.
Combination	List of peak area values used for analysis
Count	Number of samples included in QA/QC statistical metrics calculation.
CV	Coefficient of variation ($STDEV \div MEAN$) for the selected peak area combination.
Date and Time	Timestamp of analysis.
Gas	Target analyte (CH_4, N_2O, CO_2).
MEAN	Average peak areas across the combination.
Outlier	Number of samples flagged as statistical outliers across the peak area combination.
Peak Area	Represents the integrated electrical response produced by a compound as it passes through the detector.
Peak Table File (.xlsx)	A tabulated summary of data obtained from gas chromatography analysis. It lists the area under each peak in the chromatogram, which corresponds to the quantity of CH_4, N_2O, and CO_2 detected in the standard and samples.
Preparation File (.xlsx)	An Excel document that records how each batch was prepared prior to injection into the gas chromatography (GC) instrument. The file contains three worksheets namely *Preparation*, *Batch*, and *SITE ID Order*. Each worksheet provides specific details necessary for accurate and traceable sample preparation.
Preparation (worksheet)	Used to randomize gas samples for each batch by applying the RAND function.
Retention Time	Elapsed time between a sample's injection into the chromatograph and the moment a specific compound reaches a detector. It represents how long the compound spends traveling through the chromatographic column.

Sample ID	Unique identifier for each sample.
SITE ID Order (worksheet)	Describes the ambient (AMB) gases distribution within the experimental site.
Standards	Calibration standard used (e.g., AMB, 10M, 1N100M1kC, 3N500M10kC).
STDEV	Standard deviation of the peak areas.

Chapter 5: DASIG-FLUX Module

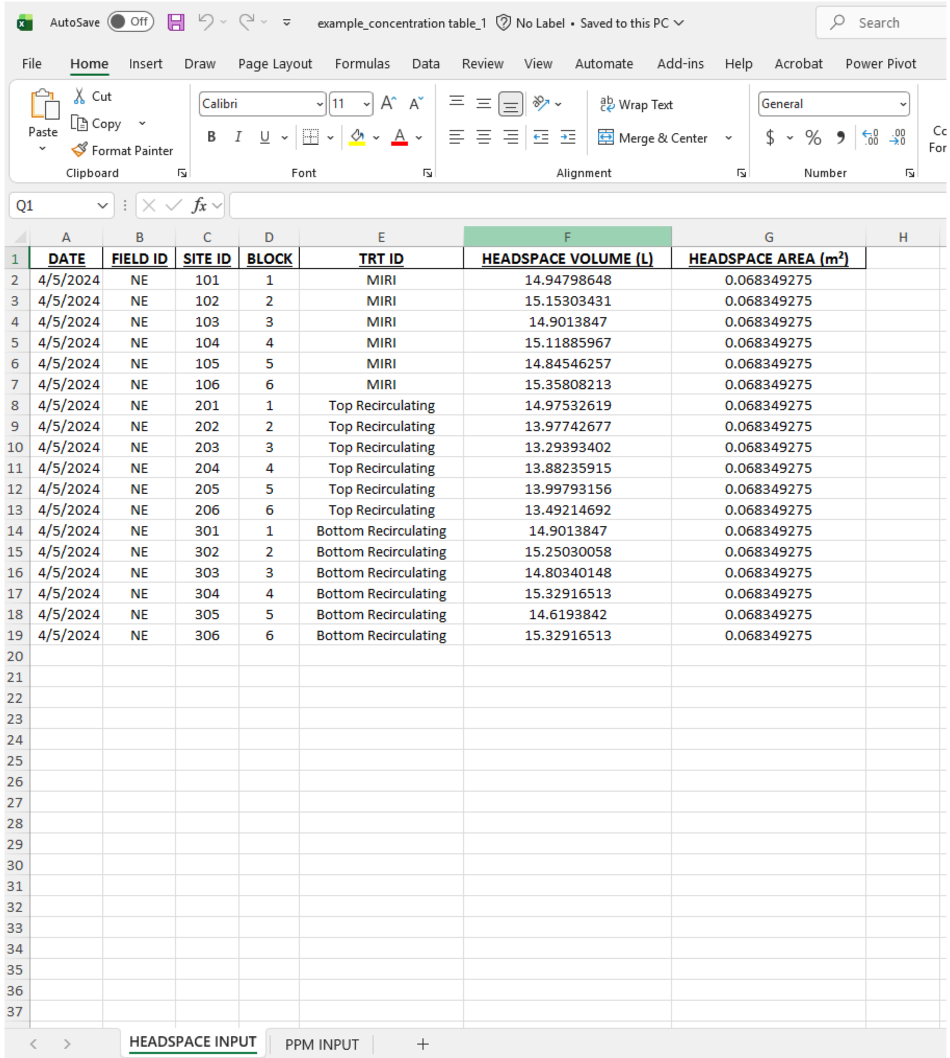
1. Overview

The DASIG-FLUX module automates the calculation of fluxes for N_2O, CH_4, and CO_2 concentration values (ppm) and converts ppm to molar quantities, with only the data points that exceed the minimum detection limits (DL) are retained for regression analysis.

The model automatically evaluates each time series using a number of quality thresholds, including R^2, DL compliance, and internal ratio checks to determine whether a linear regression or the extended HMR method is the most appropriate. The optimal method is applied to compute the final Daily Flux for each chamber event. All computed fluxes are prepared for downstream processing and are used directly as inputs to the DASIG-GWP module for total global warming potential assessment.

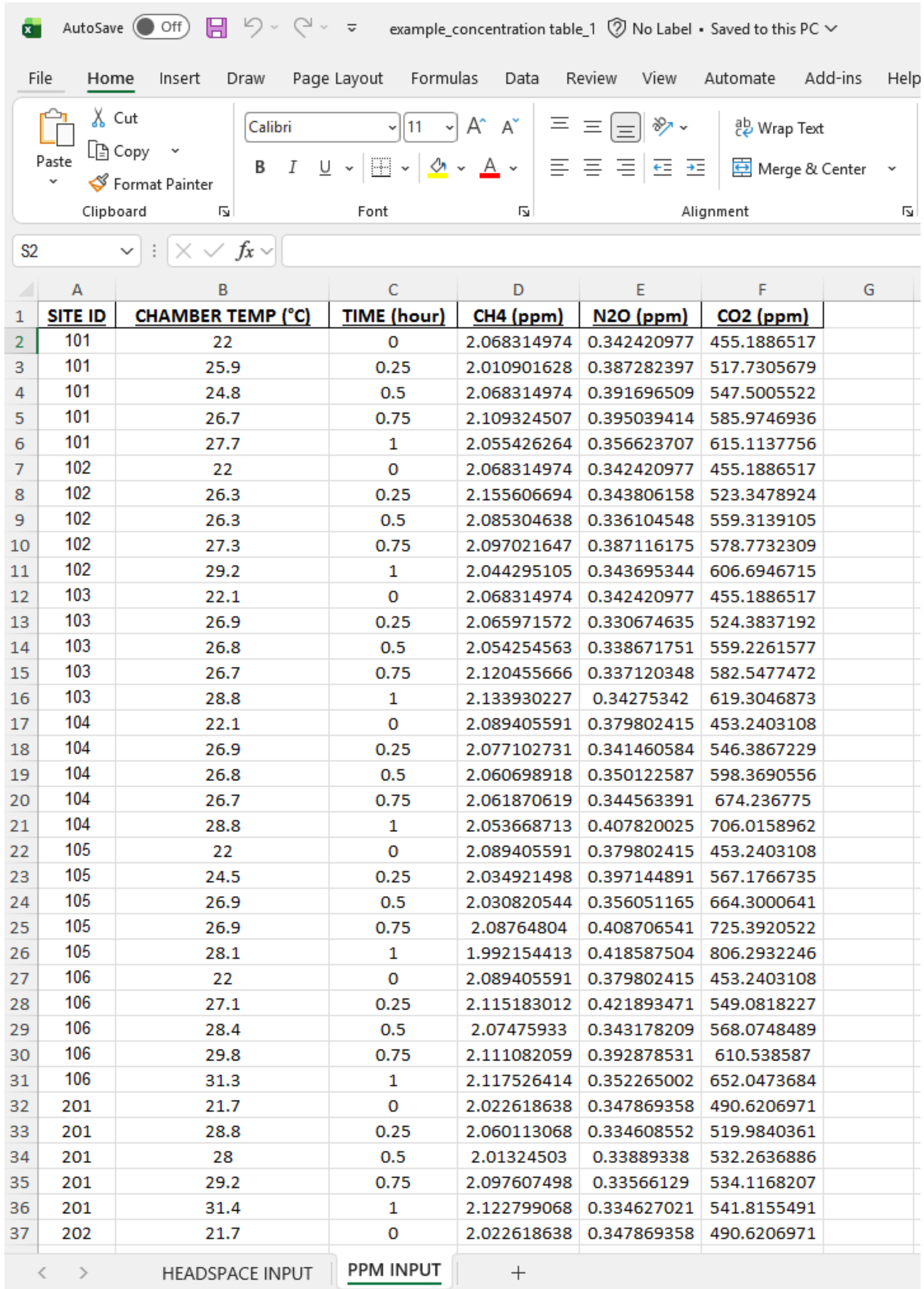
2. Quick Start

1. Prepare a *concentration table file.*
   Create an Excel file containing two sheets; *HEADSPACE INPUT* and *PPM INPUT*.
2. Verify *SITE ID* consistency
   Ensure SITE identifiers match exactly across both sheets to avoid alignment errors.



DATE	FIELD ID	SITE ID	BLOCK	TRT ID	HEADSPACE VOLUME (L)	HEADSPACE AREA (m^2)
4/5/2024	NE	101	1	MIRI	14.94798648	0.068349275
4/5/2024	NE	102	2	MIRI	15.15303431	0.068349275
4/5/2024	NE	103	3	MIRI	14.9013847	0.068349275
4/5/2024	NE	104	4	MIRI	15.11885967	0.068349275
4/5/2024	NE	105	5	MIRI	14.84546257	0.068349275
4/5/2024	NE	106	6	MIRI	15.35808213	0.068349275
4/5/2024	NE	201	1	Top Recirculating	14.97532619	0.068349275
4/5/2024	NE	202	2	Top Recirculating	13.97742677	0.068349275
4/5/2024	NE	203	3	Top Recirculating	13.29393402	0.068349275
4/5/2024	NE	204	4	Top Recirculating	13.88235915	0.068349275
4/5/2024	NE	205	5	Top Recirculating	13.99793156	0.068349275
4/5/2024	NE	206	6	Top Recirculating	13.49214692	0.068349275
4/5/2024	NE	301	1	Bottom Recirculating	14.9013847	0.068349275
4/5/2024	NE	302	2	Bottom Recirculating	15.25030058	0.068349275
4/5/2024	NE	303	3	Bottom Recirculating	14.80340148	0.068349275
4/5/2024	NE	304	4	Bottom Recirculating	15.32916513	0.068349275
4/5/2024	NE	305	5	Bottom Recirculating	14.6193842	0.068349275
4/5/2024	NE	306	6	Bottom Recirculating	15.32916513	0.068349275

Figure 5.1. Example of the *HEADSPACE INPUT* sheet in the flux input file workbook.



SITE ID	CHAMBER TEMP (°C)	TIME (hour)	CH4 (ppm)	N2O (ppm)	CO2 (ppm)
101	22	0	2.068314974	0.342420977	455.1886517
101	25.9	0.25	2.010901628	0.387282397	517.7305679
101	24.8	0.5	2.068314974	0.391696509	547.5005522
101	26.7	0.75	2.109324507	0.395039414	585.9746936
101	27.7	1	2.055426264	0.356623707	615.1137756
102	22	0	2.068314974	0.342420977	455.1886517
102	26.3	0.25	2.155606694	0.343806158	523.3478924
102	26.3	0.5	2.085304638	0.336104548	559.3139105
102	27.3	0.75	2.097021647	0.387116175	578.7732309
102	29.2	1	2.044295105	0.343695344	606.6946715
103	22.1	0	2.068314974	0.342420977	455.1886517
103	26.9	0.25	2.065971572	0.330674635	524.3837192
103	26.8	0.5	2.054254563	0.338671751	559.2261577
103	26.7	0.75	2.120455666	0.337120348	582.5477472
103	28.8	1	2.133930227	0.34275342	619.3046873
104	22.1	0	2.089405591	0.379802415	453.2403108
104	26.9	0.25	2.077102731	0.341460584	546.3867229
104	26.8	0.5	2.060698918	0.350122587	598.3690556
104	26.7	0.75	2.061870619	0.344563391	674.236775
104	28.8	1	2.053668713	0.407820025	706.0158962
105	22	0	2.089405591	0.379802415	453.2403108
105	24.5	0.25	2.034921498	0.397144891	567.1766735
105	26.9	0.5	2.030820544	0.356051165	664.3000641
105	26.9	0.75	2.08764804	0.408706541	725.3920522
105	28.1	1	1.992154413	0.418587504	806.2932246
106	22	0	2.089405591	0.379802415	453.2403108
106	27.1	0.25	2.115183012	0.421893471	549.0818227
106	28.4	0.5	2.07475933	0.343178209	568.0748489
106	29.8	0.75	2.111082059	0.392878531	610.538587
106	31.3	1	2.117526414	0.352265002	652.0473684
201	21.7	0	2.022618638	0.347869358	490.6206971
201	28.8	0.25	2.060113068	0.334608552	519.9840361
201	28	0.5	2.01324503	0.33889338	532.2636886
201	29.2	0.75	2.097607498	0.33566129	534.1168207
201	31.4	1	2.122799068	0.334627021	541.8155491
202	21.7	0	2.022618638	0.347869358	490.6206971

Figure 5.2. Example of the *PPM INPUT* sheet in flux input workbook.

3. Create *Output Folder Name*.
   Create a folder name for the results generated by the module.
4. Select *Select Working Folder.*
   Choose and create an output directory where all generated files will be saved.
5. Create *Output File Name*. This flux output file (*.xlsx*) will be used in the DASIG GWP module. Use the following information in naming the flux

output: date of sampling (yyyymmdd), field ID i.e. *20240405_NEflux* for traceability. Leave it *blank* to use the default settings (i.e. The output file name is similar to the *Output Folder Name*.

6. Designate the path/ folder where the flux output excel file will be copied/ saved in *Copy Output to Folder*.

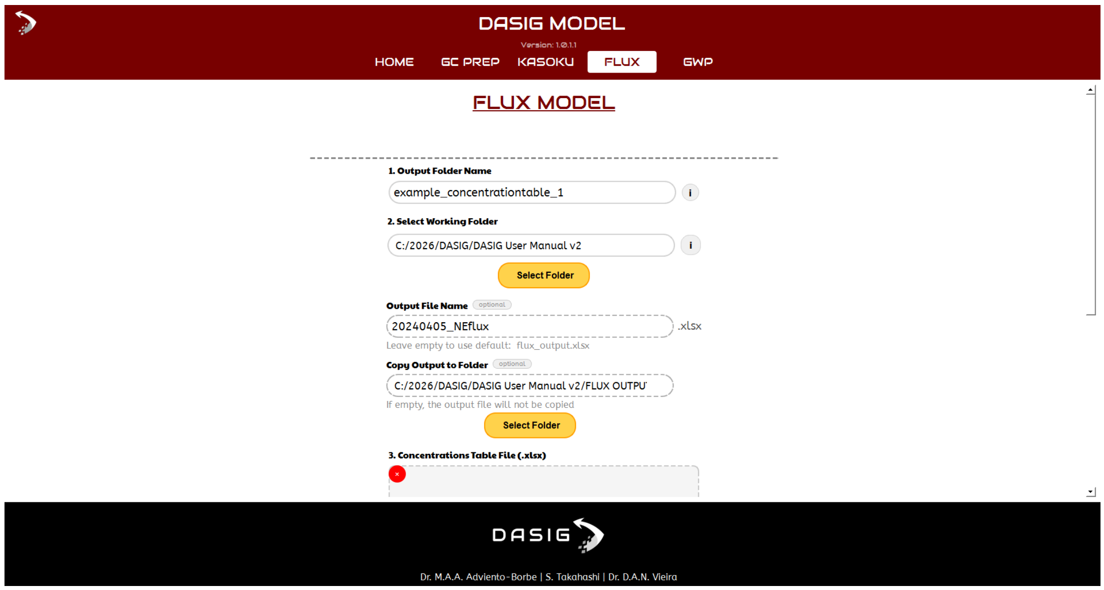


Figure 5.3. Example of *Output Folder Name*, *Working Folder*, *Output File Name* in DASIG-FLUX module.

7. Import flux input files.
   Drag and drop, or use the *Open File* button to import the flux input workbook to the *Concentrations Table File* box.
8. Input the Detection Limit for N_2O, CH_4, and CO_2.
   The DASIG-FLUX module has a default detection limit for each gas. The user may adjust the values based on their chamber application and system.
9. Run the DASIG-FLUX Module.
   Click *Start* to initiate automatic calculation of N_2O, CH_4, and CO_2 fluxes.

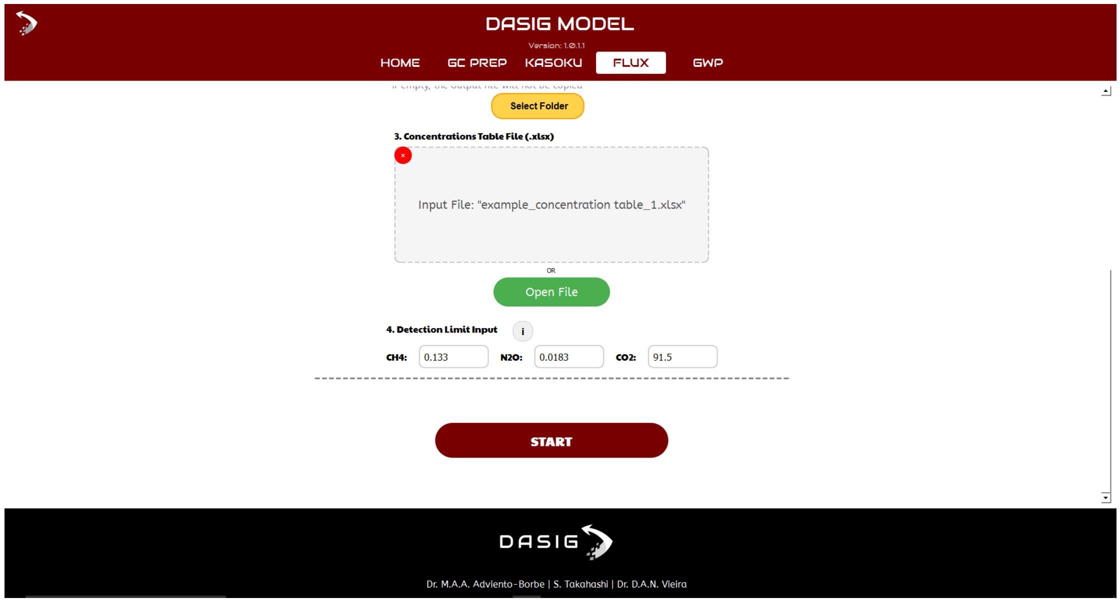


Figure 5.4. Default detection limit for each gas.

10. Input Confirmation
    Review the loaded inputs and confirm that all required fields have been correctly recognized by the interface. Click *OK* to continue. Click *CANCEL* to go back editing the module input parameters.

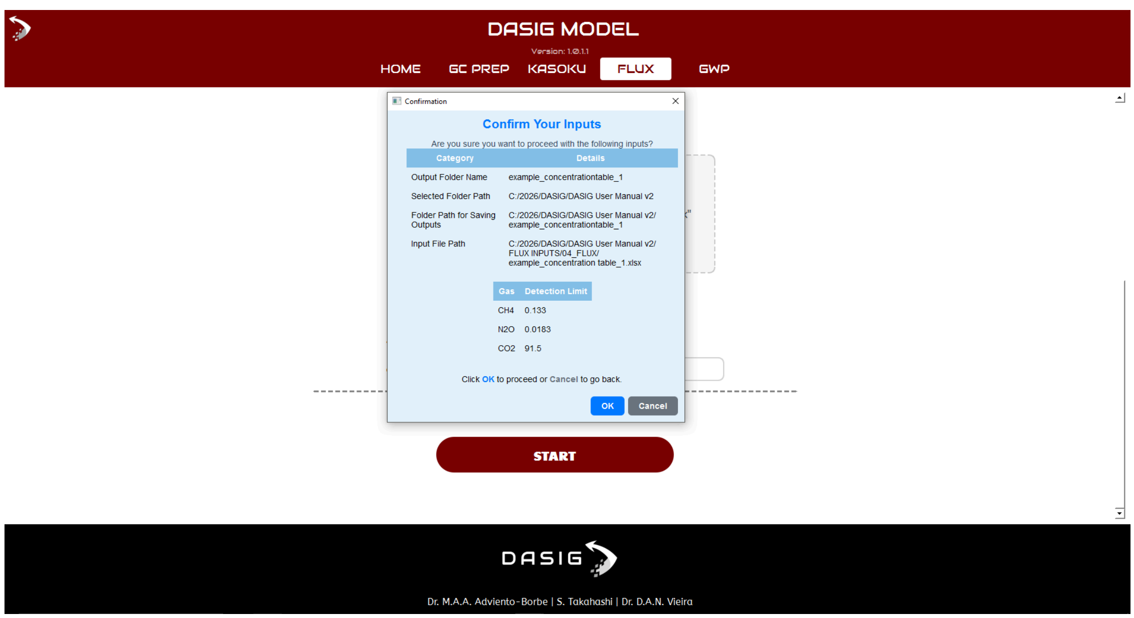


Figure 5.5. Input confirmation prompt in the DASIG-FLUX module.

11. *Select HMR Mode* Selection

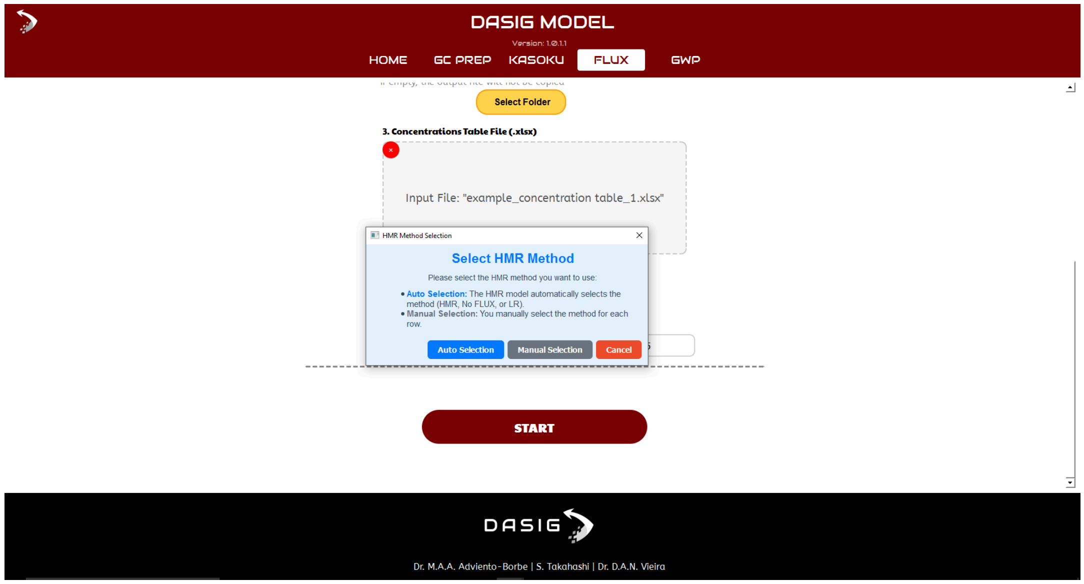


Figure 5.6. *Select HMR Method* to be used for the analysis.

Choose *HMR Method* between:

- Automatic HMR selection (*Auto Selection*), where the model apply HMR based on internal thresholds and diagnostics, or

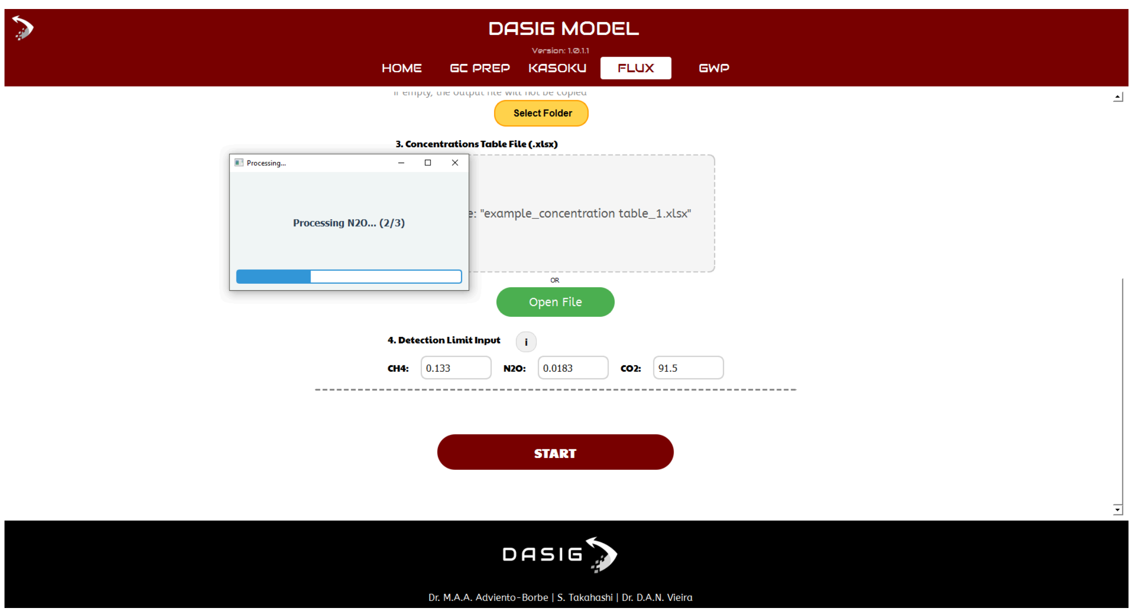


Figure 5.7. The *Auto Selection* for HMR method proceeds right away to flux calculation.

- or *Manual Selection*. Using the plot visualization to confirm non-linear patterns before enabling HMR. Click the *HMR* button until the *Data Series* reaches the last SITE ID number or 100% of all the SITE IDs are done for each gas.

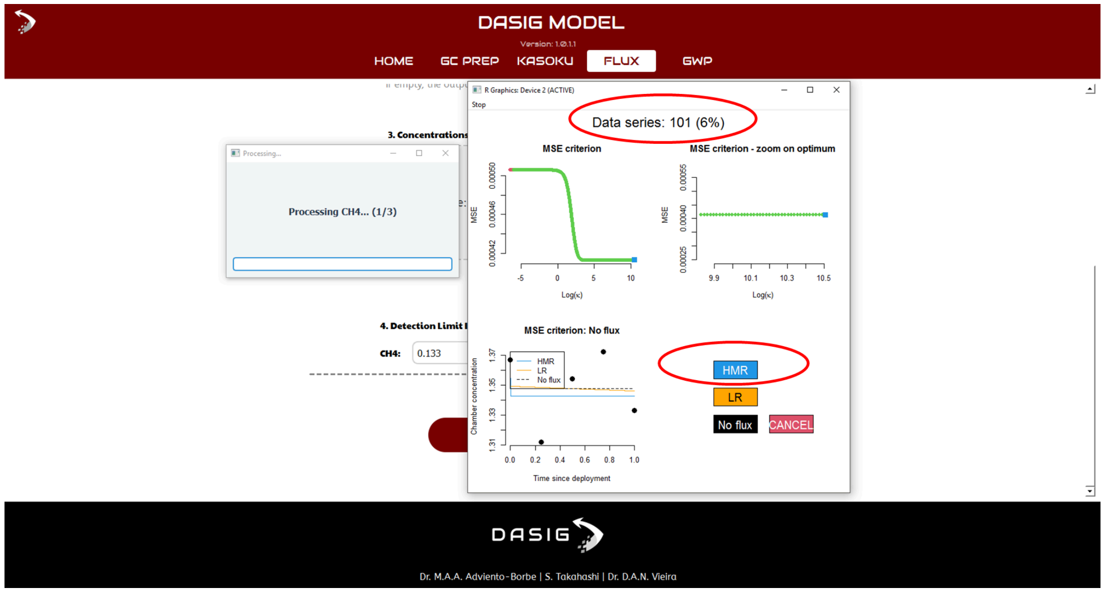


Figure 5.8. Example for *Manual Selection* for HMR analysis for CH_4 gas.

12. Program Completed.
    After the process is completed, the results will be saved in the path directory entered in step 4. Click *OK* to close the completion message.

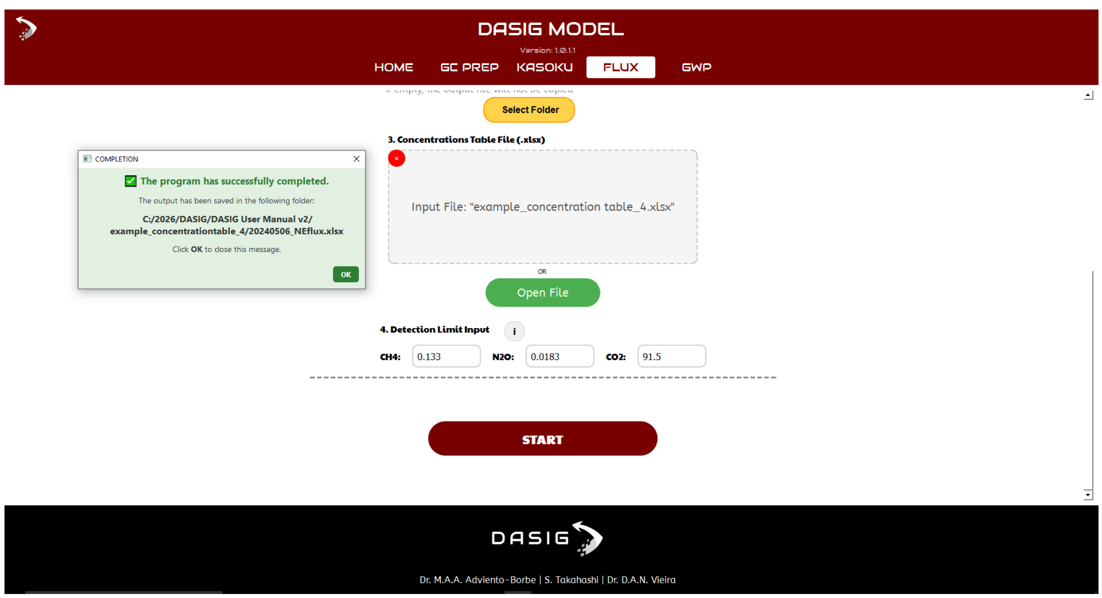


Figure 5.9. A pop-up box confirms successful program completion with no errors detected.

13. Expected Outputs
    The module generates structured outputs including the HMR analyses results of each gas and an excel workbook that consolidates all the calculations and flux results. The outputs include:

- Flux output folders and output excel files of each datasets used in the analyses.

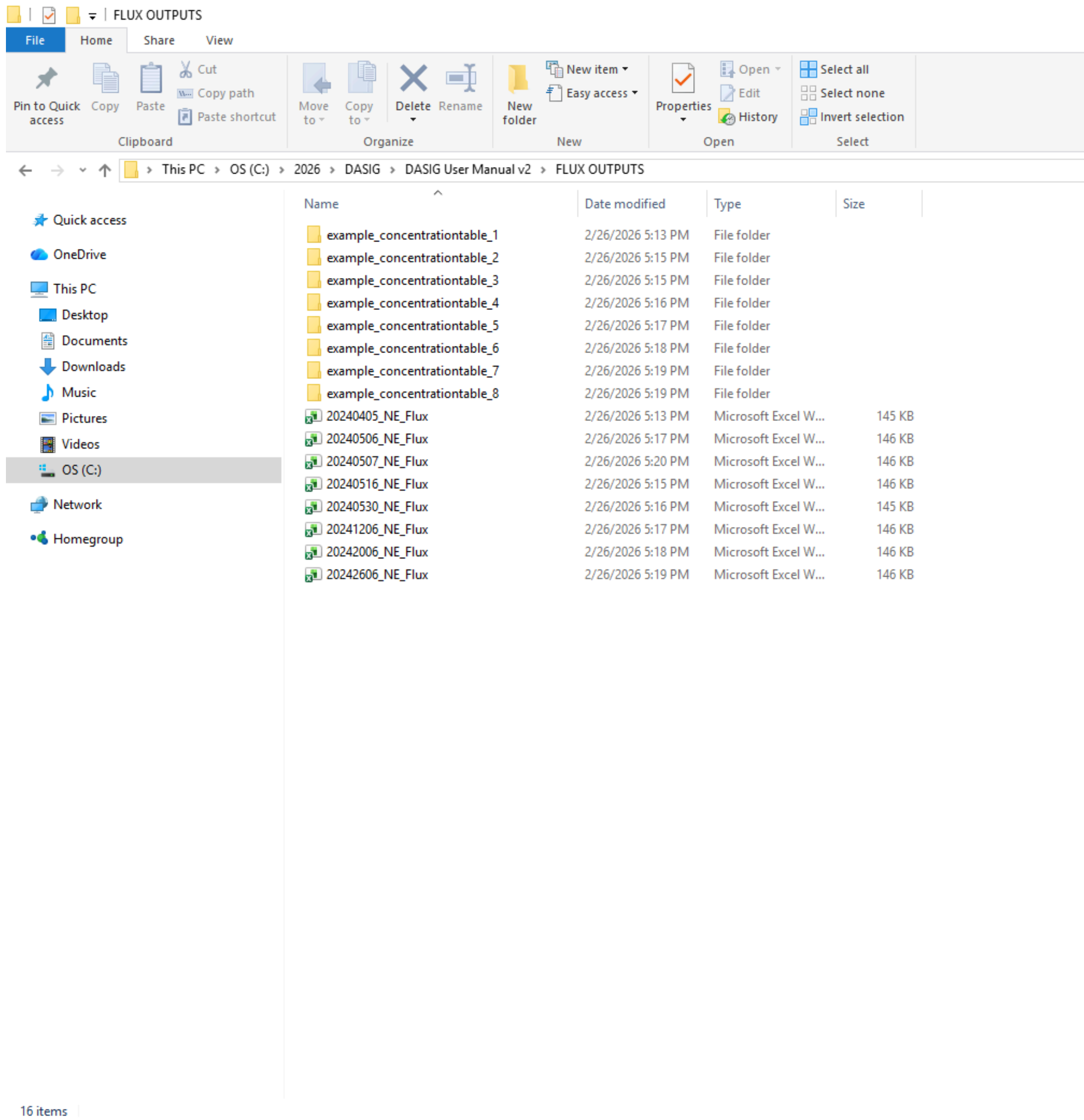


Figure 5.10. Examples of the flux output folders containing results of each data set analysis.

- Each flux output folder includes results of the HMR analyses and the flux output excel workbook for flux calculation.

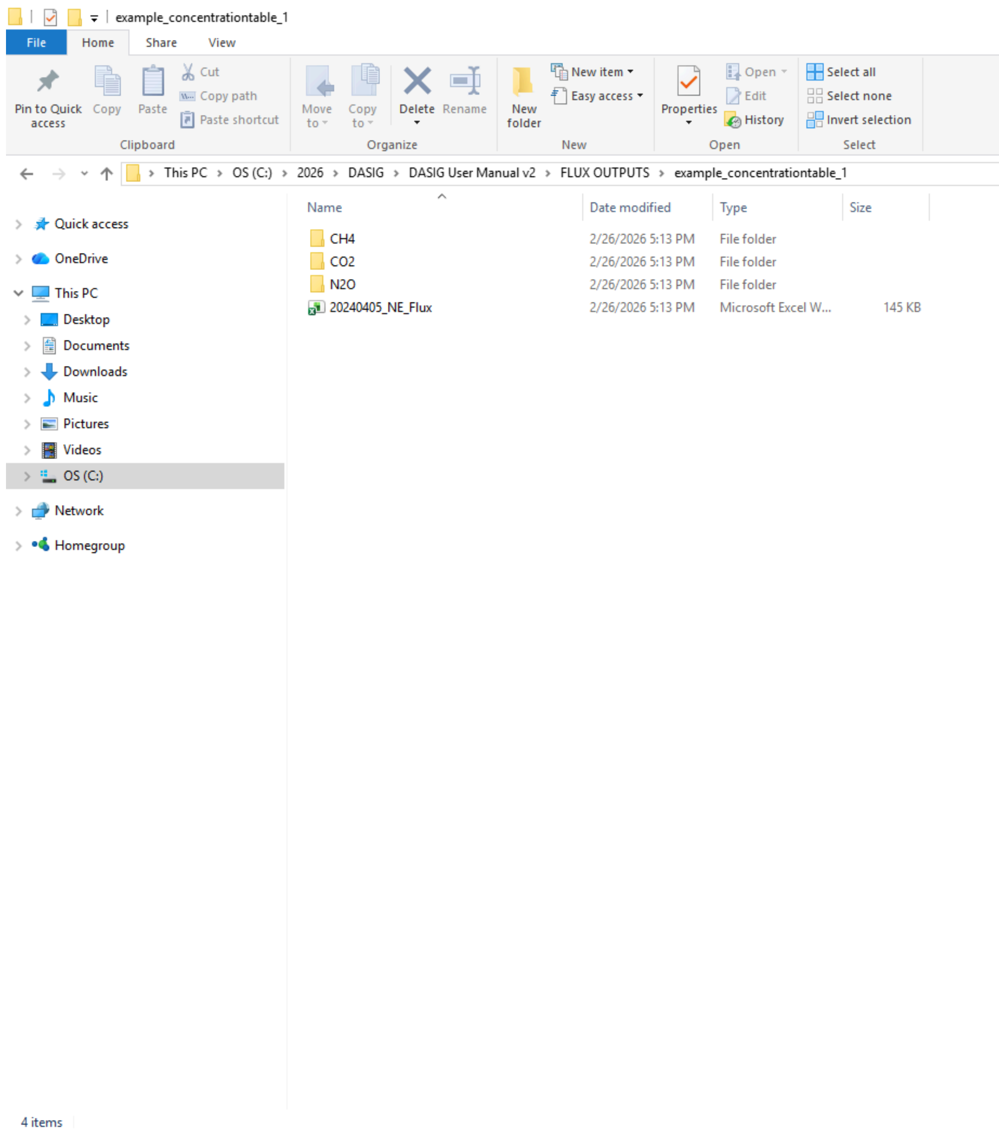


Figure 5.11. The HMR output folders and the final flux calculation in excel file.

14. Export the flux outputs (*.xlsx*) from the flux output folder if no information is provided for the *Output File Name* and *Copy Output to Folder* for the GWP module.
    Save the final results as <inputFileName>_FLUX.xlsx, For example: *example_concentration table_1_FLUX* to **20240405_NE_FLUX**.

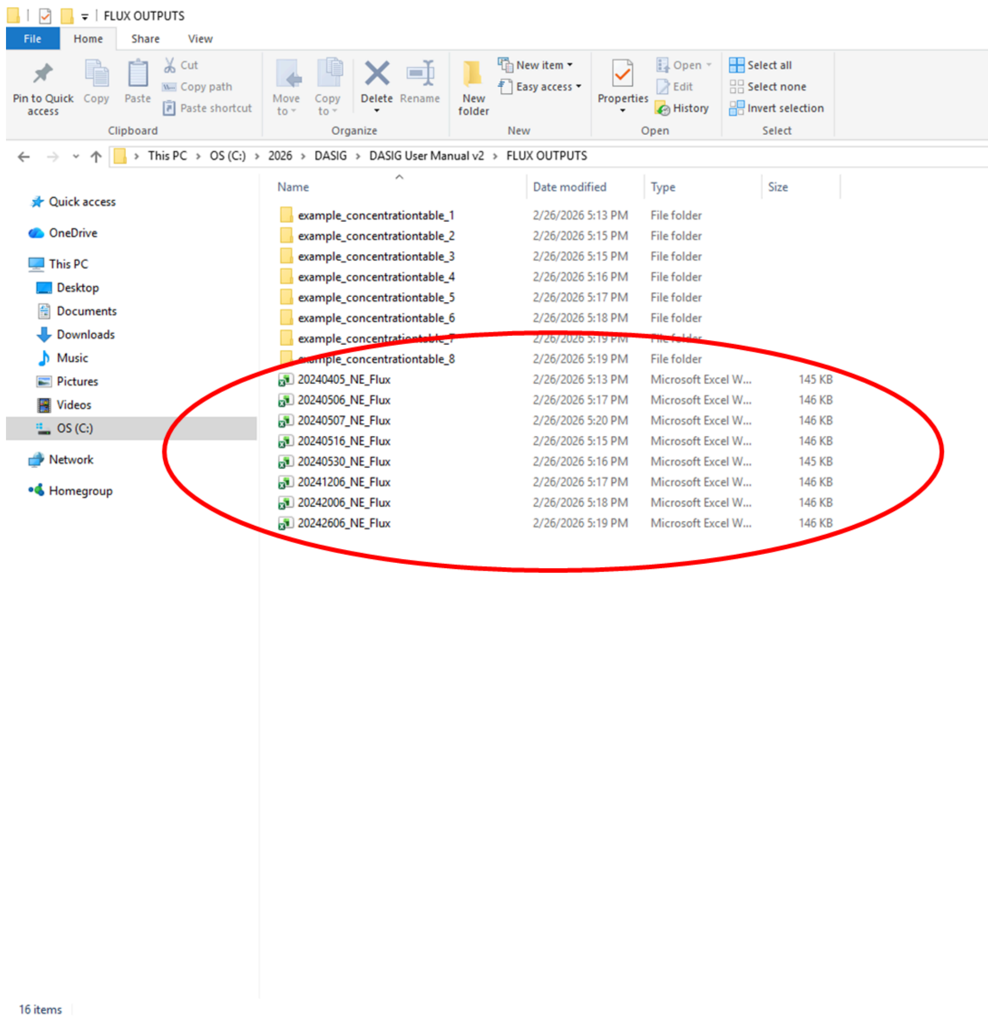


Figure 5.12. Daily flux files are exported and are ready for the GWP module.

3. Input Specification

- HEADSPACE input worksheet should contain the
  - date of sampling (DATE),
  - field ID (FIELD ID),
  - site ID (SITE ID),
  - block (BLOCK),
  - treatment ID (TRT ID),
  - headspace (HEADSPACE VOLUME (L)), and
  - HEADSPACE AREA (m^2)
- PPM input worksheet should contain
  - site ID (SITE ID),
  - chamber temperatures (CHAMBER TEMP (°C)) per time interval (TIME (hour)) and the

- N_2O, CH_4, and CO_2 concentration values (CH_4 (ppm); N_2O (ppm); CO_2 (ppm)). The concentration values used in this input worksheet are results from the KASOKU module.

4. Tips to Optimal Procedure

- *Data Preparation*
    - Format the concentrations table file: The column headers should match with the concentrations table file template to avoid headers inconsistencies (e.g. CHAMBER TEMP (°C), SITE ID, etc).
    - Verify raw input files: Ensure SITE IDs, timestamps, and gas concentrations are complete and correctly formatted before loading.Inconsistencies prevent the program from running.
    - Confirm units and calibration: Make sure gas concentrations and chamber dimensions use consistent units.
- *Module Configuration*
    - Set scientifically justified detection limits values and keep it consistent across the analysis to avoid false positives or negatives in flux outputs.
    - Review user-modifiable parameters: Confirm slope thresholds, HMR criteria, and QA flags match the logical decision standards.
    - Avoid duplicate output folder names: Use folder names that are tied with date of sampling and experiment description to ensure the module runs without interruption and data traceability (i.e. 20250405_NE).
- *Running the Module*
    - Monitor progress messages: Pay attention to warnings or QA flags that may indicate data instability.
- *Output Management*
    - Organize output folders systematically: All output files must be stored in the designated project directory using standardized naming conventions, for example:
        a. Name the concentrations table file using the date of gas sampling to easily trace the calculated flux (i.e. 20250405_NE_INPUT). Use format year month date for ease of sorting chronologically.
        b. Name the final flux excel file for GWP module use as 20250405_NE_FLUX.

5. Model Processing Flow

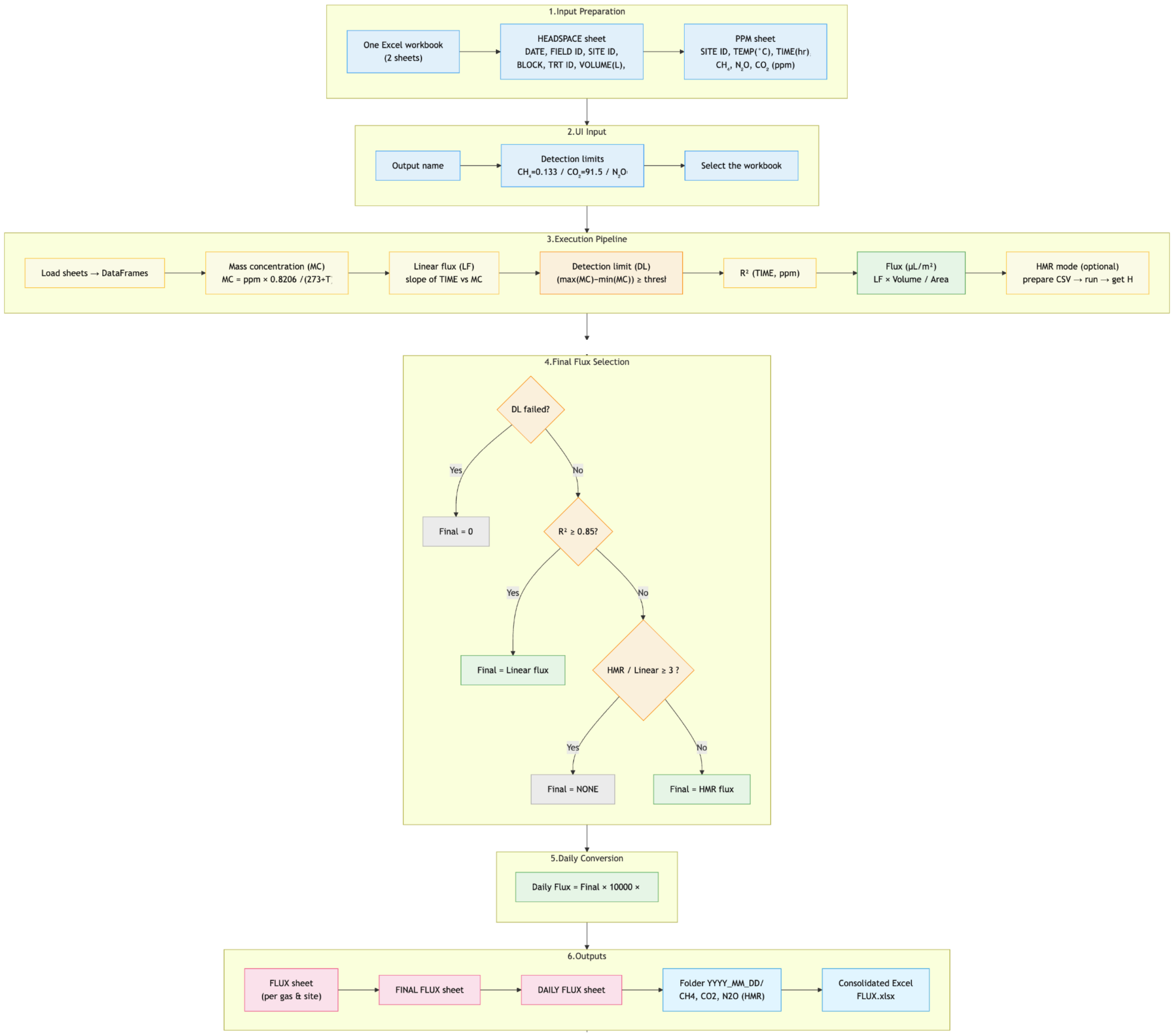


Figure 5.13. Flow diagram representing the core processing phases.

6. Quality Assurance / Quality Control (QA/QC)

The final flux selection ensures that only reliable, statistically valid flux values are retained for downstream analysis. Here's a detailed breakdown of how quality assurance and control is implemented:

- Input data preparation

Verify that all field data and gas concentration measurements collected during the sampling period are encoded and documented accurately. The module excludes any input file that does not contain the necessary variables for execution.

- User Interface (UI) parameters
  The UI parameters in the DASIG-FLUX module are highly sensitive such that it identifies duplication of *Output Folder Name*.
  User-defined detection limits for each gas may be adjusted as needed, and the entered values will be applied in the flux calculation.

- Data quality check
  The DASIG- FLUX module follows a rigorous data QA/QC for flux calculation. The system performs a defined sequence of steps to verify data accuracy prior to initiating further downstream processing.

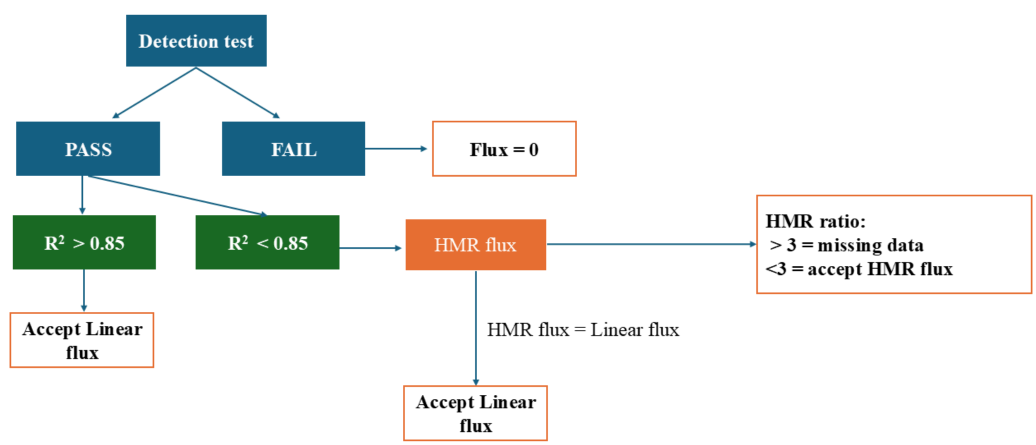


Figure 5.14. Simplified QA/QC process in accepting/ selecting calculated gas fluxes. Please refer to Figure 5.13 for the model processing flow.

1. *Detection limit check*
   Before any flux is accepted, the system checks whether the change in mass concentration (MC) over time is large enough to be considered detectable.
   (MaxMC-MinMC) $\geq$ *threshold*
   Tailored detection limits are gas-specific therefore prevent overestimation, or false positives from noise or minimal variation.

2. *Linear model evaluation, R^2*
   - If the detection limit is passed, the system evaluates the linear regression fit between time and mass concentration.
     - If $R^2 \geq 0.85$ = Linear flux
   - Indicates strong model fit and reliable flux estimate.
     - If $R^2 < 0.85 \rightarrow$ Proceed to HMR evaluation

3. *HMR vs Linear Model Comparison*
   - When the linear model is weak, the system checks whether the nonlinear HMR model provides a better estimate.
     HMR ratio = HMR flux / Linear flux
     - If HMR ratio $\geq 3 \rightarrow$ = HMR flux
   - Suggests nonlinear curvature is significant and HMR is more accurate.
     - If HMR / Linear $< 3 \rightarrow$ = missing data

     Neither model is sufficiently reliable; flux is considered as missing data.

- Output summarization
  The module generates multiple structured outputs. It organizes, preserves, and communicates the results of the flux analysis. It ensures that all processed data aligns with the input data—whether accepted, rejected, or flagged—is systematically stored and clearly labeled for downstream use, reporting, or troubleshooting.

7. Output Interpretation

Flux output folders contain calculation of fluxes in an excel file (A) and the HMR output folders (B).

A. Excel flux calculations.

The calculated fluxes are summarized in the excel file inside the flux output folder: i.e. *example_flux_input_1_FLUX*. This excel file will be used as the input file for GWP analysis. This file is composed of five sheets specifically: It contains *HEADSPACE INPUT* and *PPM INPUT* sheets.

- The *FLUX* sheet is composed of all the data from the concentrations table file (Quick start 1), mass concentrations in a given volume (μg/L), calculated linear flux of each gas, quality assurance (QA) / quality control (QC) steps: detection score of each gas (*PASS*/ *FAIL*), linearity of concentration (ppm) of each gas over an hour time (R^2), and the calculated flux in mass concentrations of each gas in a given area (µg/m^2) in each SITE ID.

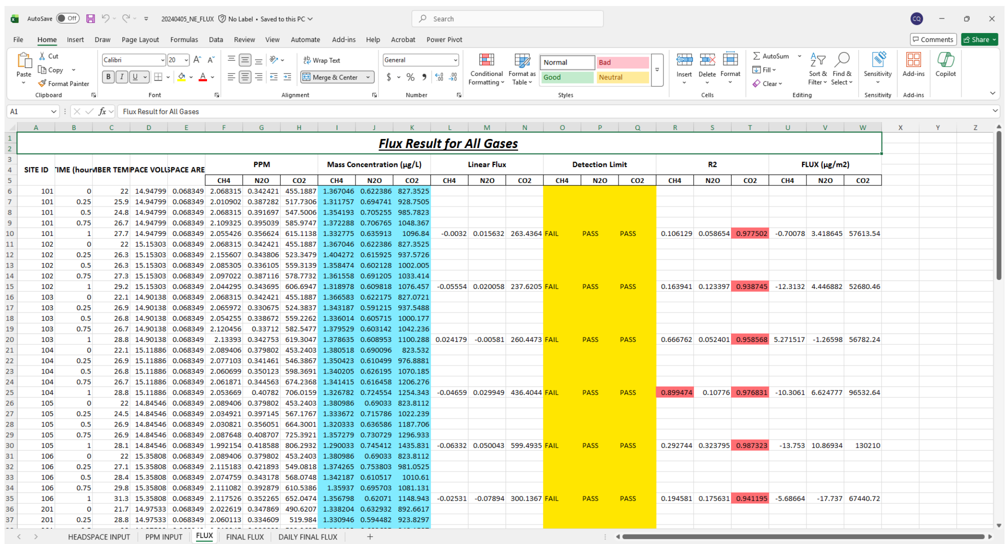


Figure 5.15. Example of the FLUX sheet for all the sample and standard gases showing the mass concentrations, linear flux, detection score, linearity of gas concentrations (R^2), and calculated flux per SiteID.

- The *FLUX* sheet contains all intermediate calculations prior to final QA/QC filtering. It serves as the foundational record of all computations and must be retained for verification and audit purposes. This sheet includes:

    a. Mass concentration (MC, µg/L)
    It is the volume of gas at sampling temperature. The calculation of MC uses the Ideal Gas Law at chamber air temperature measured during each sampling event and the molar mass of each gas (CH_4 = 16; N_2O = 44; CO_2 = 44 g/mol) to calculate the mass concentration (µg N_2O, CO_2 or CH_4 L^{-1}).
    MC (µg/L) = ((ppm*molar mass)/0.08206)/(273+chamber temperature).

    b. Linear Flux

Linear flux is the slope of mass concentration (ppm) over time. This data indicates whether there is an increase of concentration of gases over time which will be used for further flux calculation (Flux (μg/m2)). The CH_4 and CO_2 ppm follows a linear increase over time, while N_2O does not.

c. Detection limit (DL, μg/L)
Detection limit is calculated from the calibrations of the analytical columns used in gas chromatograph instruments using the standard gases and minimum gas flux detection using the chamber set-up. The detection limit determines whether the difference between the maximum and minimum concentration of each gas (CH_4, N_2O, CO_2) over a set time period is significant. If the change exceeds the detection limit, the result is *PASS*; otherwise, *FAIL*.

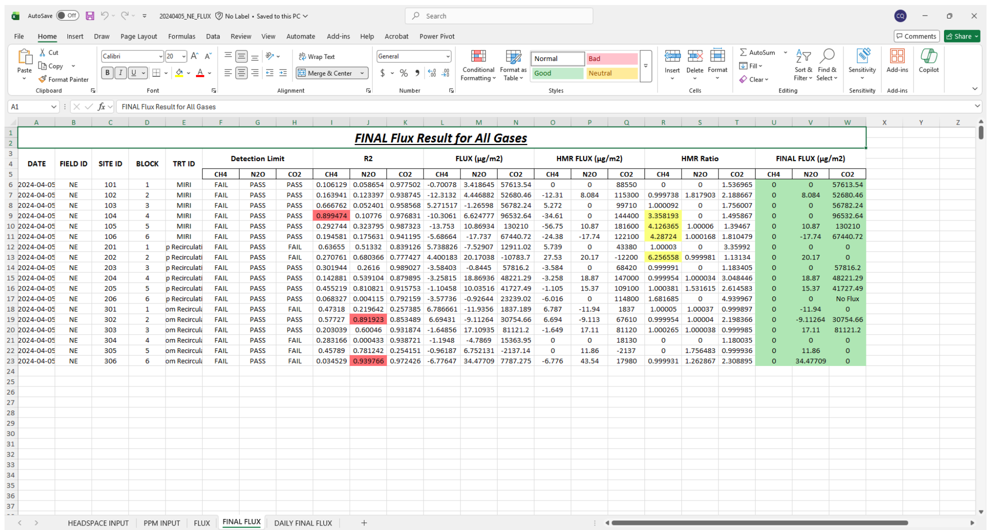
(MaxMC-MinMC) $\geq$ threshold

PASS = gas concentration changed enough to be detected;
FAIL = '0'; gas concentration change was too small, falling below the instrument's chamber and chamber's sensitivity threshold.

d. Regression of concentration values (ppm) over time, R^2
Fluxes of CH_4, CO_2 and N_2O (μg/m^2) were estimated from the linear increase of gas concentration over time.

$R^2 \geq 0.85$ - *Linear flux: Flux (μg/m2)*
$R^2 \leq 0.85$, or non-linear, gas fluxes (*HMR flux*) were calculated in R (R Development Core Team, 2019) using the HMR script. A visual inspection of all flux curves were shown to avoid erroneous data points, or low signal-to-noise ratios that may overestimate the HMR fluxes (Figure ? *Manual Selection*, step 9).

- The *FINAL FLUX* sheet contains the flux values that pass or fail the QA/QC decision logic. It shows the fluxes accepted based on detection limits and model-fit criteria, zero fluxes assigned due to failed detection limit, missing values for fluxes that fail both linear and HMR criteria, and model origin labels (Linear or HMR) for accepted fluxes. This sheet represents the validated dataset for statistical analysis, reporting, and interpretation. It includes:



FINAL Flux Result for All Gases

DATE	FIELD ID	SITE ID	BLOCK	TRT ID	Detection Limit			R2			FLUX (µg/m2)			HMR FLUX (µg/m2)			HMR Ratio			FINAL FLUX (µg/m2)		
					CH4	N2O	CO2	CH4	N2O	CO2	CH4	N2O	CO2	CH4	N2O	CO2	CH4	N2O	CO2	CH4	N2O	CO2
2024-04-05	NE	101	1	MIRI	FAIL	PASS	PASS	0.106129	0.058654	0.977502	-0.70078	3.418645	57613.54	0	0	88550	0	0	1.536965	0	0	57613.54
2024-04-05	NE	102	2	MIRI	FAIL	PASS	PASS	0.163941	0.123397	0.938745	-12.3132	4.446882	52680.46	-12.31	8.084	115300	0.999738	1.817903	2.188667	0	8.084	52680.46
2024-04-05	NE	103	3	MIRI	FAIL	PASS	PASS	0.666762	0.052401	0.958568	5.271517	-1.26598	56782.24	5.272	0	99710	1.000092	0	1.756007	0	0	56782.24
2024-04-05	NE	104	4	MIRI	FAIL	PASS	PASS	0.899474	0.10776	0.976831	-10.3061	6.624777	96532.64	-34.61	0	144400	3.358193	0	1.495867	0	0	96532.64
2024-04-05	NE	105	5	MIRI	FAIL	PASS	PASS	0.292744	0.323795	0.987323	-13.753	10.86934	130210	-56.75	10.87	181600	4.126365	1.00006	1.39467	0	10.87	130210
2024-04-05	NE	106	6	MIRI	FAIL	PASS	PASS	0.194581	0.175631	0.941195	-5.68664	-17.737	67440.72	-24.38	-17.74	122100	4.28724	1.000168	1.810479	0	-17.74	67440.72
2024-04-05	NE	201	1	p Recirculati	FAIL	PASS	FAIL	0.63655	0.51332	0.839126	5.738826	-7.52907	12911.02	5.739	0	43380	1.00003	0	3.35992	0	0	0
2024-04-05	NE	202	2	p Recirculati	FAIL	PASS	FAIL	0.270761	0.680366	0.777427	4.400183	20.17038	-10783.7	27.53	20.17	-12200	6.256558	0.999981	1.13134	0	20.17	0
2024-04-05	NE	203	3	p Recirculati	FAIL	PASS	PASS	0.301944	0.2616	0.989027	-3.58403	-0.8445	57816.2	-3.584	0	68420	0.999991	0	1.183405	0	0	57816.2
2024-04-05	NE	204	4	p Recirculati	FAIL	PASS	PASS	0.142881	0.539104	0.879895	-3.25815	18.86936	48221.29	-3.258	18.87	147000	0.999954	1.000034	3.048446	0	18.87	48221.29
2024-04-05	NE	205	5	p Recirculati	FAIL	PASS	PASS	0.455219	0.810821	0.915753	-1.10458	10.03516	41727.49	-1.105	15.37	109100	1.000381	1.531615	2.614583	0	15.37	41727.49
2024-04-05	NE	206	6	p Recirculati	FAIL	PASS	PASS	0.068327	0.004115	0.792159	-3.57736	-0.92644	23239.02	-6.016	0	114800	1.681685	0	4.939967	0	0	No Flux
2024-04-05	NE	301	1	om Recircula	FAIL	PASS	FAIL	0.47318	0.219642	0.257385	6.786661	-11.9356	1837.189	6.787	-11.94	1837	1.00005	1.00037	0.999897	0	-11.94	0
2024-04-05	NE	302	2	om Recircula	FAIL	PASS	PASS	0.57727	0.891923	0.853489	6.69431	-9.11264	30754.66	6.694	-9.113	67610	0.999954	1.00004	2.198366	0	-9.11264	30754.66
2024-04-05	NE	303	3	om Recircula	FAIL	PASS	PASS	0.203039	0.60046	0.931874	-1.64856	17.10935	81121.2	-1.649	17.11	81120	1.000265	1.000038	0.999985	0	17.11	81121.2
2024-04-05	NE	304	4	om Recircula	FAIL	PASS	FAIL	0.283166	0.000433	0.938721	-1.1948	-4.7869	15363.95	0	0	18130	0	0	1.180035	0	0	0
2024-04-05	NE	305	5	om Recircula	FAIL	PASS	FAIL	0.45789	0.781242	0.254151	-0.96187	6.752131	-2137.14	0	11.86	-2137	0	1.756483	0.999936	0	11.86	0
2024-04-05	NE	306	6	om Recircula	FAIL	PASS	FAIL	0.034529	0.939766	0.972426	-6.77647	34.47709	7787.275	-6.776	43.54	17980	0.999931	1.262867	2.308895	0	34.47709	0

Figure 5.16. Flux results for all gases showing the R^2 and calculated HMR ratio for identifying the acceptable FINAL FLUX (µg/m²). red- means the R^2 is $\geq$ 0.85; yellow - means HMR ratio is > 3; green - means *Final Flux (µg/m2)* based from QA/QC

e. Flux (µg/m²)

Flux rate is the change of the mass concentration per change in time in a given chamber volume in an enclosed area. It is calculated using the formula:

F=V*(dC)/A*(dt)

where:

F = gas flux rate, mg m^{-2} min^{-1}

V = volume of headspace, m^3

A = area covered of static chamber, m^2

dC = change in gas concentration, mg m^{-3}

dC= gas concentration at time t3 - gas concentration at time t1

dt = change in time, min

dt = time t2 - time t1

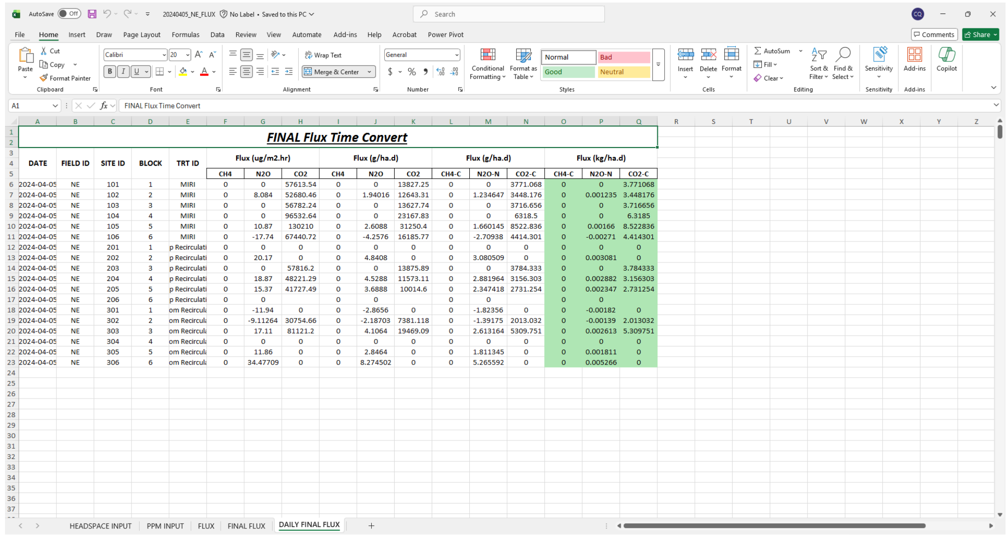
f. HMR Flux

It is the gas emission or uptake rate calculated using the Hutchinson–Mosier Regression approach, a statistical method designed to handle the curved (non-linear) changes in gas concentration that often occur inside static chambers. Instead of assuming a simple linear increase in concentration, HMR fits a curve to the chamber data, giving a more realistic estimate of how quickly gases like N_2O, CO_2, or CH_4 are moving between the soil and the atmosphere.

g. HMR Ratio
HMR flux / Linear flux.
It is a data-quality metric used to judge whether the concentration-versus-time data collected inside the chamber is stable enough to justify calculating a linear flux.
If the concentration mass is non-linear, the HMR ratio is calculated. It is the ratio of HMR flux / Linear flux.
If HMR flux = Linear Flux, use the Linear flux for further analysis
If HMR ratio > 3 = 'missing data'
If HMR ratio < 3 = use HMR flux for further analysis

h. Final Flux (µg/m^2)
Selected calculated flux that passed the QA/QC. This flux will be used for final flux conversions.

- The *DAILY FINAL FLUX* sheet provides daily emission rates derived from the final accepted flux values. It applies the appropriate conversion factors to standardize fluxes across sampling intervals and chamber deployment durations. This output supports temporal comparisons and integration into ecological or agronomic models.



FINAL Flux Time Convert

DATE	FIELD ID	SITE ID	BLOCK	TRT ID	Flux (ug/m2.hr)			Flux (g/ha.d)			Flux (g/ha.d)			Flux (kg/ha.d)		
					CH4	N2O	CO2	CH4	N2O	CO2	CH4-C	N2O-N	CO2-C	CH4-C	N2O-N	CO2-C
2024-04-05	NE	101	1	MIRI	0	0	57613.54	0	0	13827.25	0	0	3771.068	0	0	3.771068
2024-04-05	NE	102	2	MIRI	0	8.084	52680.46	0	1.94016	12643.31	0	1.234647	3448.176	0	0.001235	3.448176
2024-04-05	NE	103	3	MIRI	0	0	56782.24	0	0	13627.74	0	0	3716.656	0	0	3.716656
2024-04-05	NE	104	4	MIRI	0	0	96532.64	0	0	23167.83	0	0	6318.5	0	0	6.3185
2024-04-05	NE	105	5	MIRI	0	10.87	130210	0	2.6088	31250.4	0	1.660145	8522.836	0	0.00166	8.522836
2024-04-05	NE	106	6	MIRI	0	-17.74	67440.72	0	-4.2576	16185.77	0	-2.70938	4414.301	0	-0.00271	4.414301
2024-04-05	NE	201	1	p Recirculati	0	0	0	0	0	0	0	0	0	0	0	0
2024-04-05	NE	202	2	p Recirculati	0	20.17	0	0	4.8408	0	0	3.080509	0	0	0.003081	0
2024-04-05	NE	203	3	p Recirculati	0	0	57816.2	0	0	13875.89	0	0	3784.333	0	0	3.784333
2024-04-05	NE	204	4	p Recirculati	0	18.87	48221.29	0	4.5288	11573.11	0	2.881964	3156.303	0	0.002882	3.156303
2024-04-05	NE	205	5	p Recirculati	0	15.37	41727.49	0	3.6888	10014.6	0	2.347418	2731.254	0	0.002347	2.731254
2024-04-05	NE	206	6	p Recirculati	0	0		0	0		0	0		0	0	
2024-04-05	NE	301	1	om Recircula	0	-11.94	0	0	-2.8656	0	0	-1.82356	0	0	-0.00182	0
2024-04-05	NE	302	2	om Recircula	0	-9.11264	30754.66	0	-2.18703	7381.118	0	-1.39175	2013.032	0	-0.00139	2.013032
2024-04-05	NE	303	3	om Recircula	0	17.11	81121.2	0	4.1064	19469.09	0	2.613164	5309.751	0	0.002613	5.309751
2024-04-05	NE	304	4	om Recircula	0	0	0	0	0	0	0	0	0	0	0	0
2024-04-05	NE	305	5	om Recircula	0	11.86	0	0	2.8464	0	0	1.811345	0	0	0.001811	0
2024-04-05	NE	306	6	om Recircula	0	34.47709	0	0	8.274502	0	0	5.265592	0	0	0.005266	0

Figure 5.17. DASIG-Flux module outputs (*DAILY FINAL FLUX*) after passing the QA/QC steps.

i. Flux (μg/m^2.hr)
The flux (μg/m^2.hr) is the change of the mass concentration per change in time (hour). This is the calculated flux after passing the QA/QC process.

j. Flux (g/ha.d)
The flux (μg/m^2.hr) is converted to mass concentration in grams per hectare per day in the compound form of the gases CH_4, N_2O and CO_2.

k. Flux (g/ha.d) in elemental form
This is the flux in grams per hectare per day in elemental form (g CH_4-C; g N_2O-N; g CO_2-C per ha.d). This data is the final unit used for daily flux and will be used for GWP analyses.
Using elemental mass allows direct comparison of how much carbon or nitrogen is actually being emitted. For example:
Carbon - 12 g atomic mass
Hydrogen - 1 g atomic mass
Nitrogen - 14 g atomic mass
Oxygen - 16 g atomic mass

CH_4: 12 C+ (1*4) = 16 g

N_2O: (14*2) + 16 = 44 g
CO_2: 12 + (16*2) = 44 g

$$CH4\ compound\ form: \frac{gCH4}{ha\ d}\ x\ \frac{12\ C}{16\ CH4} = CH4\ elemetal\ form\ \frac{g\ CH4 - C}{ha\ d}$$

$$N2O\ compound\ form: \frac{gN2O}{ha\ d}\ x\ \frac{28\ N}{44\ N2O} = N2O\ elemetal\ form\ \frac{g\ N2O - N}{ha\ d}$$

$$CO2\ compound\ form: \frac{gCO2}{ha\ d}\ x\ \frac{12\ C}{44\ CO2} = CO2\ elemetal\ form\ \frac{g\ CO2 - C}{ha\ d}$$

1. Flux (kg/ha.d) in elemental form.
   The flux is converted to kilograms per hectare per day.

B. The HMR Output Folder (Nonlinear Model Files)

If HMR modeling is enabled, the workflow generates a date-stamped folder. These files are organized by date and gas type to ensure full reproducibility of nonlinear model runs.

The results from HMR analyses of each gas (i.e. CH_4). The *CH_4* CSV file contains the HEADSPACE INPUT and PPM INPUT data (Figure), and the raw and summary of HMR and linear model analyses results.

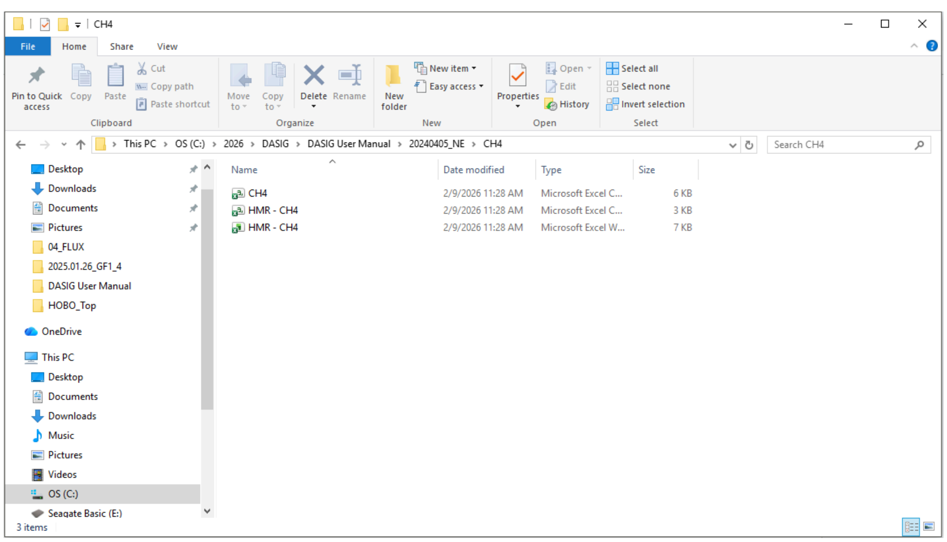


Figure 5.18. The outputs from the HMR analyses are specific for each gas.

- HMR data files (input data)

These are CSV files containing five columns with SITE IDs with respective chamber volumes, chamber areas, time points and gas concentrations.

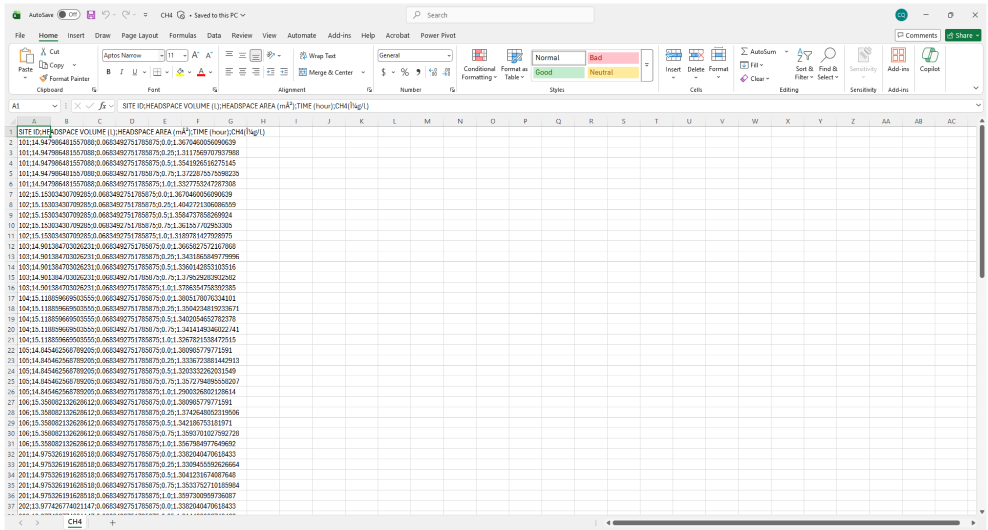


Figure 5.19. Example of the input data in (*CH4.csv*) in each gas output folder.

- HMR output files contain the raw and summary of linear and HMR flux results calculated using the HMR R script.

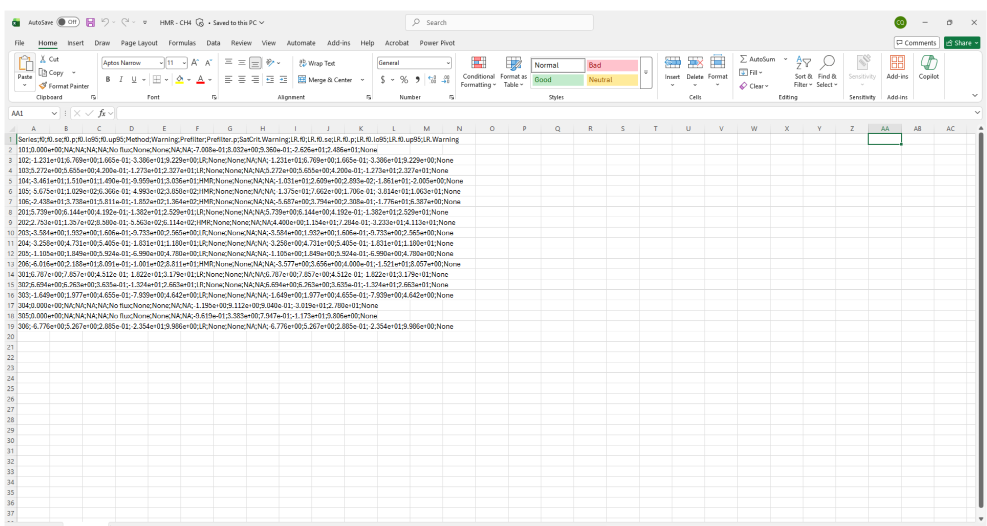
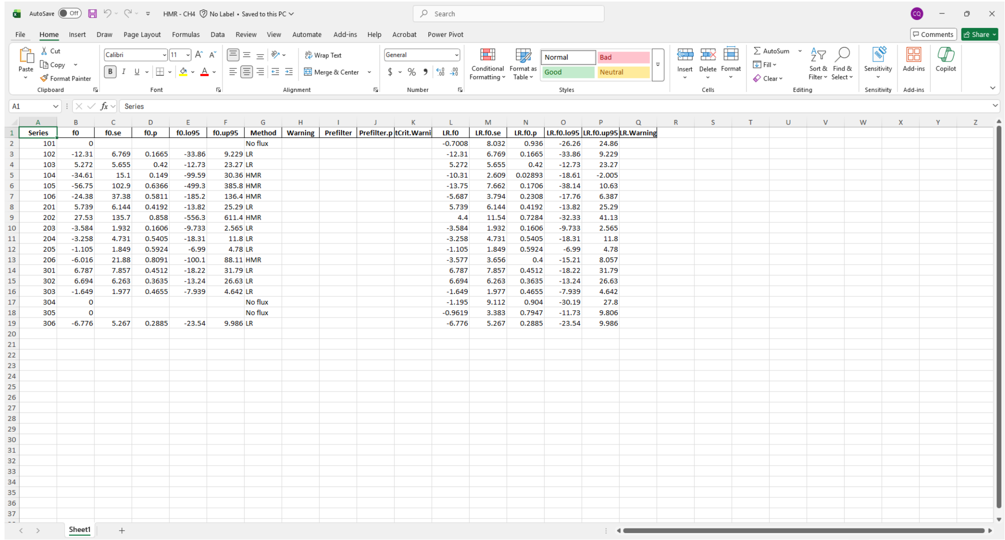


Figure 5.20. HMR results containing the linear and HMR flux results (*HMR - CH4.csv*).



Series	f0	f0.se	f0.p	f0.lo95	f0.up95	Method
101	0					No flux
102	-12.31	6.769	0.1665	-33.86	9.229	LR
103	5.272	5.655	0.42	-12.73	23.27	LR
104	-34.61	15.1	0.149	-99.59	30.36	HMR
105	-56.75	102.9	0.6366	-499.3	385.8	HMR
106	-24.38	37.38	0.5811	-185.2	136.4	HMR
201	5.739	6.144	0.4192	-13.82	25.29	LR
202	27.53	135.7	0.858	-556.3	611.4	HMR
203	-3.584	1.932	0.1606	-9.733	2.565	LR
204	-3.258	4.731	0.5405	-18.31	11.8	LR
205	-1.105	1.849	0.5924	-6.99	4.78	LR
206	-6.016	21.88	0.8091	-100.1	88.11	HMR
301	6.787	7.857	0.4512	-18.22	31.79	LR
302	6.694	6.263	0.3635	-13.24	26.63	LR
303	-1.649	1.977	0.4655	-7.939	4.642	LR
304	0					No flux
305	0					No flux
306	-6.776	5.267	0.2885	-23.54	9.986	LR

Series	Warning	Prefilter	Prefilter.p	tCrit.Warni	LR.f0	LR.f0.se	LR.f0.p	LR.f0.lo95	LR.f0.up95	LR.Warning
101					-0.7008	8.032	0.936	-26.26	24.86	
102					-12.31	6.769	0.1665	-33.86	9.229	
103					5.272	5.655	0.42	-12.73	23.27	
104					-10.31	2.609	0.02893	-18.61	-2.005	
105					-13.75	7.662	0.1706	-38.14	10.63	
106					-5.687	3.794	0.2308	-17.76	6.387	
201					5.739	6.144	0.4192	-13.82	25.29	
202					4.4	11.54	0.7284	-32.33	41.13	
203					-3.584	1.932	0.1606	-9.733	2.565	
204					-3.258	4.731	0.5405	-18.31	11.8	
205					-1.105	1.849	0.5924	-6.99	4.78	
206					-3.577	3.656	0.4	-15.21	8.057	
301					6.787	7.857	0.4512	-18.22	31.79	
302					6.694	6.263	0.3635	-13.24	26.63	
303					-1.649	1.977	0.4655	-7.939	4.642	
304					-1.195	9.112	0.904	-30.19	27.8	
305					-0.9619	3.383	0.7947	-11.73	9.806	
306					-6.776	5.267	0.2885	-23.54	9.986	

Figure 5.21. Summary of HMR results (*HMR - CH4.xlx*).

The HMR output files includes the following parameters:

Parameters	Description
f0	The estimated flux.
f0.se	The standard error of the estimated flux.
f0.p	The p-value for the null hypothesis of zero flux.
f0.lo95	The p-value for the null hypothesis of zero flux.
f0.up95	The upper end-point of the 95%-confidence interval for the flux.
Method Warning	The method used for estimating the flux ('HMR', 'LR', 'No flux' or 'None').
Prefilter	The prefiltering classification ('Signal', 'Noise' or 'None').
Prefilter.p	The prefiltering p-value.
SatCrit.Warning	A character string with a warning message if flux limiting is active.

LR.f0	The flux estimated by linear regression. (Only present if LR.always=TRUE.)
LR.f0.se	The standard error of the flux estimated by linear regression. (Only present if LR.always=TRUE.)
LR.f0.p	The standard error of the flux estimated by linear regression. (Only present if LR.always=TRUE.)
LR.f0.lo95	The lower end-point of the 95%-confidence interval for the flux calculated by linear regression. (Only present if LR.always=TRUE.)
LR.f0.up95	The upper end-point of the 95%-confidence interval for the flux calculated by linear regression. (Only present if LR.always=TRUE.)
LR.Warning	A character string with a warning message if linear regression estimated a negative predeployment concentration. (Only present if LR.always=TRUE.)

Source: Pederson et al., 2010 (http://www.r-project.org)

8. Troubleshooting

Issue: Column name differences and/ sheet name differences
Column headers and/ sheet names in the concentrations table file do not match the template.

Impact: The DASIG-FLUX module identifies the error in the input file and will not proceed to data processing until necessary edits are done (i.e. inconsistent column headers i.e. *oC* in chamber temperature should be ℃, and sheet name PPM should be PPM INPUT).

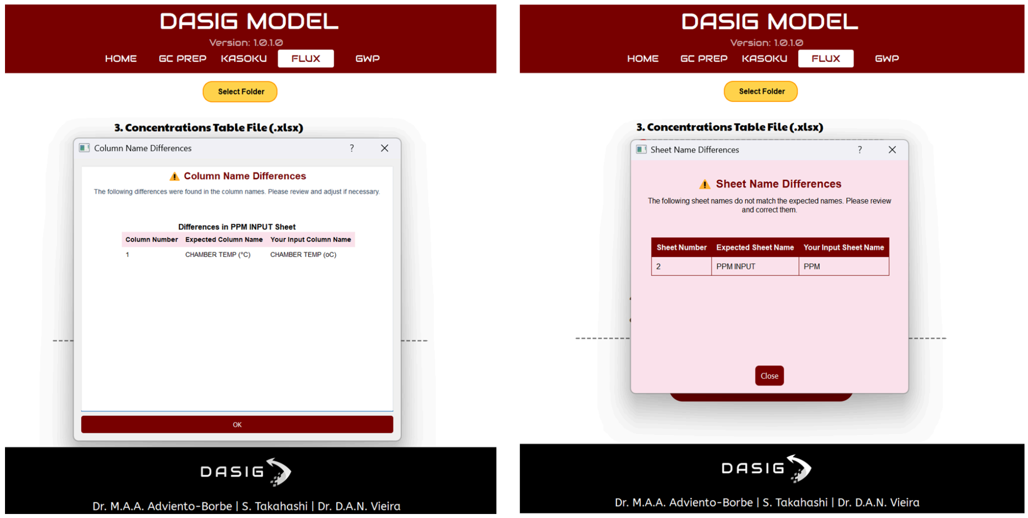
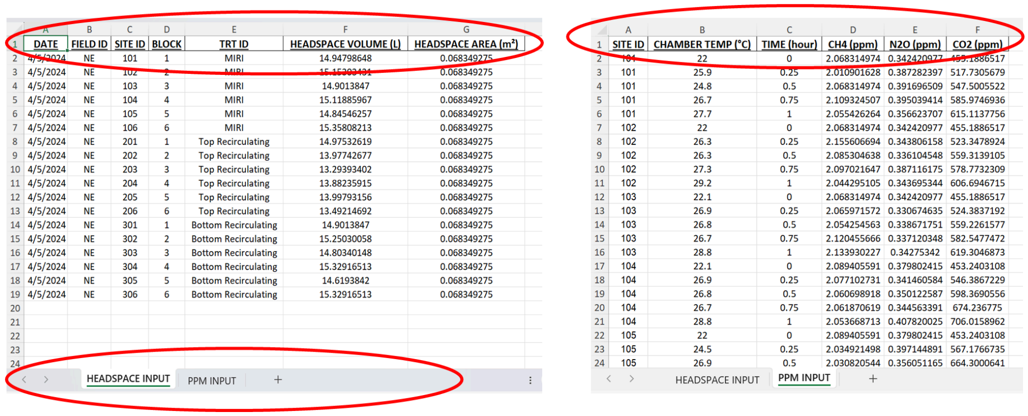


Figure 5.22. Errors with inconsistent column and sheet names.

Resolution: Column header and sheet names for the concentrations table file should match the headers in the concentrations table file template.



	A	B	C	D	E	F	G
1	DATE	FIELD ID	SITE ID	BLOCK	TRT ID	HEADSPACE VOLUME (L)	HEADSPACE AREA (m²)
2	4/5/2024	NE	101	1	MIRI	14.94798648	0.068349275
3	4/5/2024	NE	102	2	MIRI	[illegible]	0.068349275
4	4/5/2024	NE	103	3	MIRI	14.9013847	0.068349275
5	4/5/2024	NE	104	4	MIRI	15.11885967	0.068349275
6	4/5/2024	NE	105	5	MIRI	14.84546257	0.068349275
7	4/5/2024	NE	106	6	MIRI	15.35808213	0.068349275
8	4/5/2024	NE	201	1	Top Recirculating	14.97532619	0.068349275
9	4/5/2024	NE	202	2	Top Recirculating	13.97742677	0.068349275
10	4/5/2024	NE	203	3	Top Recirculating	13.29393402	0.068349275
11	4/5/2024	NE	204	4	Top Recirculating	13.88235915	0.068349275
12	4/5/2024	NE	205	5	Top Recirculating	13.99793156	0.068349275
13	4/5/2024	NE	206	6	Top Recirculating	13.49214692	0.068349275
14	4/5/2024	NE	301	1	Bottom Recirculating	14.9013847	0.068349275
15	4/5/2024	NE	302	2	Bottom Recirculating	15.25030058	0.068349275
16	4/5/2024	NE	303	3	Bottom Recirculating	14.80340148	0.068349275
17	4/5/2024	NE	304	4	Bottom Recirculating	15.32916513	0.068349275
18	4/5/2024	NE	305	5	Bottom Recirculating	14.6193842	0.068349275
19	4/5/2024	NE	306	6	Bottom Recirculating	15.32916513	0.068349275
20							
21							
22							
23							
24							

HEADSPACE INPUT | PPM INPUT

	A	B	C	D	E	F
1	SITE ID	CHAMBER TEMP (°C)	TIME (hour)	CH4 (ppm)	N2O (ppm)	CO2 (ppm)
2	101	22	0	2.068314974	0.342420977	455.1886517
3	101	25.9	0.25	2.010901628	0.387282397	517.7305679
4	101	24.8	0.5	2.068314974	0.391696509	547.5005522
5	101	26.7	0.75	2.109324507	0.395039414	585.9746936
6	101	27.7	1	2.055426264	0.356623707	615.1137756
7	102	22	0	2.068314974	0.342420977	455.1886517
8	102	26.3	0.25	2.155606694	0.343806158	523.3478924
9	102	26.3	0.5	2.085304638	0.336104548	559.3139105
10	102	27.3	0.75	2.097021647	0.387116175	578.7732309
11	102	29.2	1	2.044295105	0.343695344	606.6946715
12	103	22.1	0	2.068314974	0.342420977	455.1886517
13	103	26.9	0.25	2.065971572	0.330674635	524.3837192
14	103	26.8	0.5	2.054254563	0.338671751	559.2261577
15	103	26.7	0.75	2.120455666	0.337120348	582.5477472
16	103	28.8	1	2.133930227	0.34275342	619.3046873
17	104	22.1	0	2.089405591	0.379802415	453.2403108
18	104	26.9	0.25	2.077102731	0.341460584	546.3867229
19	104	26.8	0.5	2.060698918	0.350122587	598.3690556
20	104	26.7	0.75	2.061870619	0.344563391	674.236775
21	104	28.8	1	2.053668713	0.407820025	706.0158962
22	105	22	0	2.089405591	0.379802415	453.2403108
23	105	24.5	0.25	2.034921498	0.397144891	567.1766735
24	105	26.9	0.5	2.030820544	0.356051165	664.3000641

HEADSPACE INPUT | PPM INPUT

Figure 5.23. Column headings and sheet names of input files should be consistent.

Issue: Duplicate *Output Folder Name.*

Impact: The module will not execute when an *Output Folder Name* is duplicated.

Resolution: Provide a different name for the output folder.

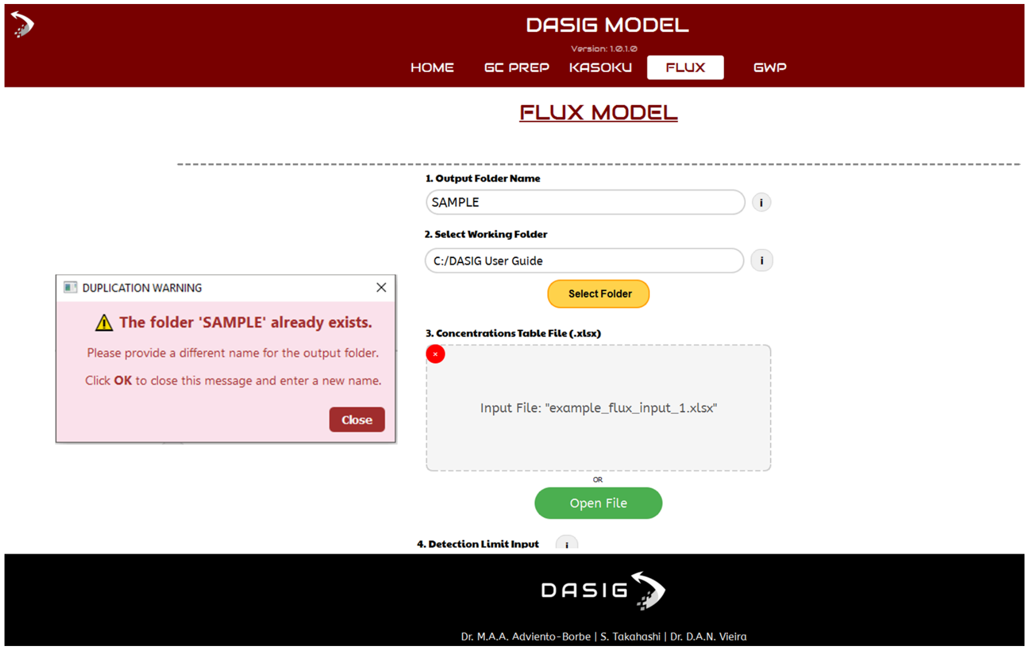
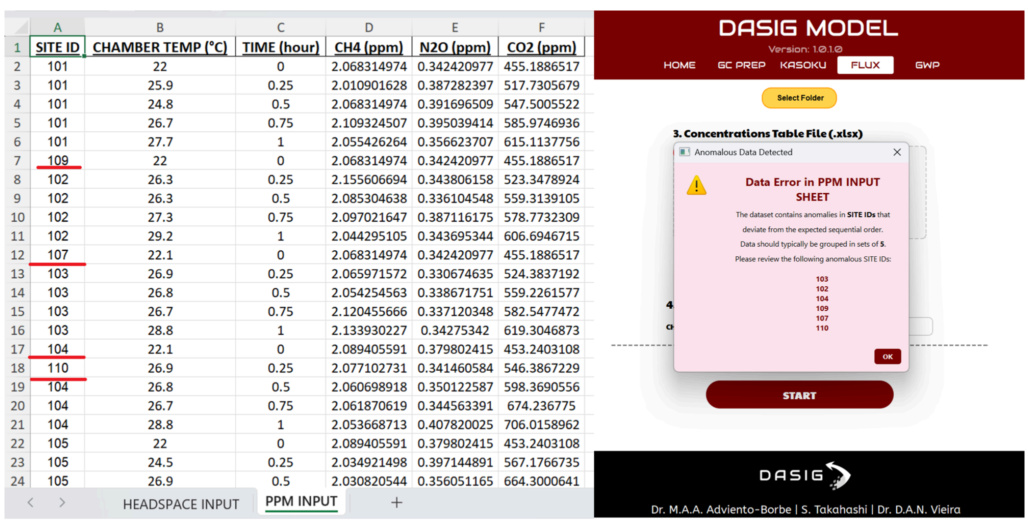


Figure 5.24. A warning indicating a duplicate *Output Folder Name*.

Issue: Data error in *PPM INPUT SHEET*

Impact: Anomalous data prevents the module from generating output.

Resolution: Make sure to check and provide the correct SITE IDs based on the experimental design. The DASIG-FLUX module will identify anomalous SITE IDs to check and modify.



SITE ID	CHAMBER TEMP (°C)	TIME (hour)	CH4 (ppm)	N2O (ppm)	CO2 (ppm)
101	22	0	2.068314974	0.342420977	455.1886517
101	25.9	0.25	2.010901628	0.387282397	517.7305679
101	24.8	0.5	2.068314974	0.391696509	547.5005522
101	26.7	0.75	2.109324507	0.395039414	585.9746936
101	27.7	1	2.055426264	0.356623707	615.1137756
109	22	0	2.068314974	0.342420977	455.1886517
102	26.3	0.25	2.155606694	0.343806158	523.3478924
102	26.3	0.5	2.085304638	0.336104548	559.3139105
102	27.3	0.75	2.097021647	0.387116175	578.7732309
102	29.2	1	2.044295105	0.343695344	606.6946715
107	22.1	0	2.068314974	0.342420977	455.1886517
103	26.9	0.25	2.065971572	0.330674635	524.3837192
103	26.8	0.5	2.054254563	0.338671751	559.2261577
103	26.7	0.75	2.120455666	0.337120348	582.5477472
103	28.8	1	2.133930227	0.34275342	619.3046873
104	22.1	0	2.089405591	0.379802415	453.2403108
110	26.9	0.25	2.077102731	0.341460584	546.3867229
104	26.8	0.5	2.060698918	0.350122587	598.3690556
104	26.7	0.75	2.061870619	0.344563391	674.236775
104	28.8	1	2.053668713	0.407820025	706.0158962
105	22	0	2.089405591	0.379802415	453.2403108
105	24.5	0.25	2.034921498	0.397144891	567.1766735
105	26.9	0.5	2.030820544	0.356051165	664.3000641

Figure 5.25. Inconsistent <u>SITE IDs</u> in PPM INPUT sheet. The DASIG-FLUX module identifies data error and the action needed to resolve the issue.

Issue: Missing *<u>SITE IDs</u>* detected in the HEADPSPACE INPUT sheet.

Impact: The issue prevents the model from running properly.

Resolution: Provide correct and consistent <u>SITE IDs</u> found in both the HEADSPACE INPUT and PPM INPUT sheets.

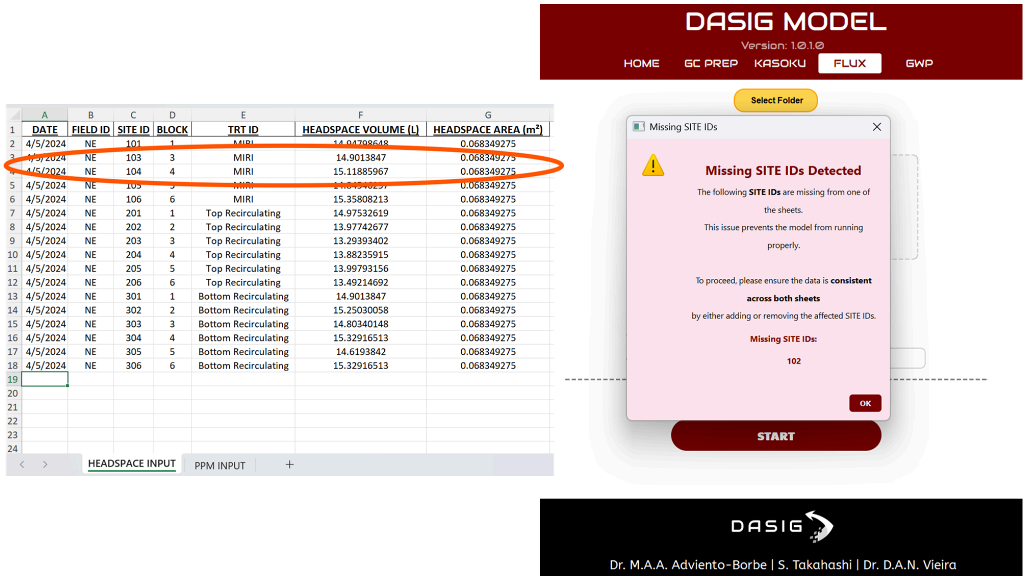


Figure 5.26. Error with missing <u>SITE IDs</u> detected by DASIG-FLUX module.

Issue: Missing data input.

Impact: If the user chooses to '*Proceed*', the module will not generate outputs.

Resolution: Address the missing values in the input file.

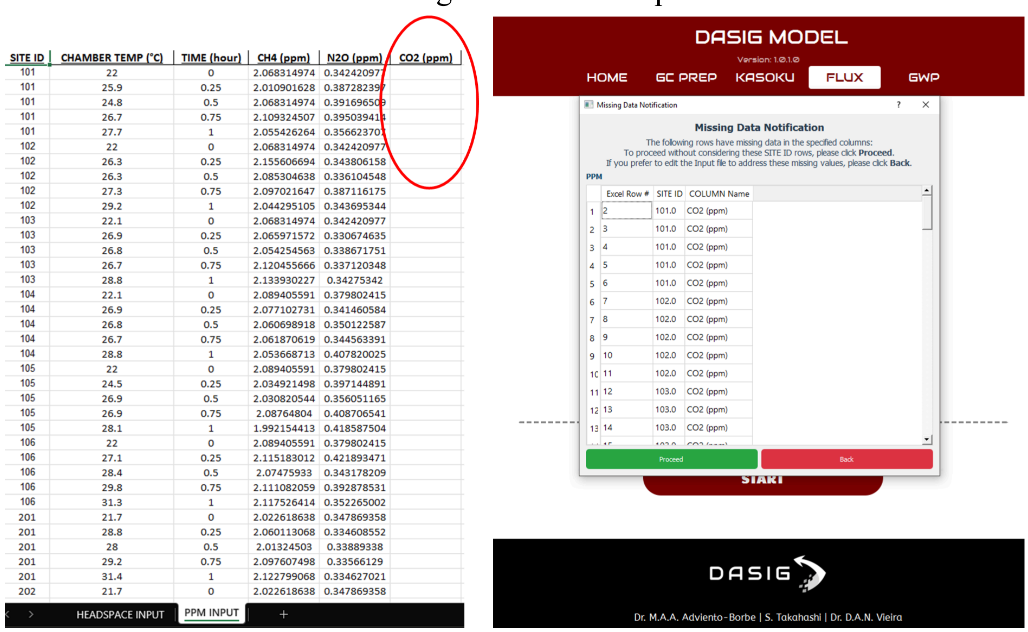


Figure 5.27. A warning indicating a missing input data.

Issue: Incorrect TRT IDs in HEADSPACE INPUT sheet.

Impact: Incorrect TRT IDs will cause inconsistencies in GWP calculation. The DASIG-FLUX module will run however, it will affect the GWP outputs.

Resolution: Check and provide consistent TRT IDs and other information in the input file throughout the Flux analyses.

FINAL Flux Time Convert

DATE	FIELD ID	SITE ID	BLOCK	TRT ID	Flux (ug/m2.hr)			Flux (g/ha.d)			Flux (g/ha.d)			Flux (kg/ha.d)		
					CH4	N2O	CO2	CH4	N2O	CO2	CH4-C	N2O-N	CO2-C	CH4-C	N2O-N	CO2-C
2024-04-05	NE	101	1	MIRI	0	0	57613.54	0	0	13827.25	0	0	3771.068	0	0	3.771068
2024-04-05	NE	102	2	MRI	0	8.084	52680.46	0	1.94016	12643.31	0	1.234647	3448.176	0	0.001235	3.448176
2024-04-05	NE	103	3	MIRI	0	0	56782.24	0	0	13627.74	0	0	3716.656	0	0	3.716656
2024-04-05	NE	104	4	MIRI	0	0	96532.64	0	0	23167.83	0	0	6318.5	0	0	6.3185
2024-04-05	NE	105	5	MIRI	0	10.87	130210	0	2.6088	31250.4	0	1.660145	8522.836	0	0.00166	8.522836
2024-04-05	NE	106	6	MIRI	0	-17.74	67440.72	0	-4.2576	16185.77	0	-2.70938	4414.301	0	-0.00271	4.414301
2024-04-05	NE	201	1	› Recirculat	0	0	0	0	0	0	0	0	0	0	0	0
2024-04-05	NE	202	2	› Recirculat	0	20.17	0	0	4.8408	0	0	3.080509	0	0	0.003081	0
2024-04-05	NE	203	3	› Recirculat	0	0	57816.2	0	0	13875.89	0	0	3784.333	0	0	3.784333
2024-04-05	NE	204	4	› Recirculat	0	18.87	48221.29	0	4.5288	11573.11	0	2.881964	3156.303	0	0.002882	3.156303
2024-04-05	NE	205	5	› Recirculat	0	15.37	41727.49	0	3.6888	10014.6	0	2.347418	2731.254	0	0.002347	2.731254
2024-04-05	NE	206	6	› Recirculat	0	0		0	0		0	0		0	0	
2024-04-05	NE	301	1	›m Recircul	0	-11.94	0	0	-2.8656	0	0	-1.82356	0	0	-0.00182	0
2024-04-05	NE	302	2	›m Recircul	0	-9.11264	30754.66	0	-2.18703	7381.118	0	-1.39175	2013.032	0	-0.00139	2.013032
2024-04-05	NE	303	3	›m Recircul	0	17.11	81121.2	0	4.1064	19469.09	0	2.613164	5309.751	0	0.002613	5.309751
2024-04-05	NE	304	4	›m Recircul	0	0	0	0	0	0	0	0	0	0	0	0
2024-04-05	NE	305	5	›m Recircul	0	11.86	0	0	2.8464	0	0	1.811345	0	0	0.001811	0
2024-04-05	NE	306	6	›m Recircul	0	34.47709	0	0	8.274502	0	0	5.265592	0	0	0.005266	0

HEADSPACE INPUT | PPM INPUT | FLUX | FINAL FLUX | DAILY FINAL FLUX

Figure 5.28. Inconsistent TRT ID in HEADSPACE INPUT sheet from the flux input file will create errors in GWP outputs.

Issue: Data error: *Invalid flux output values*

Impact: Zero CO_2-C flux values are not valid under field conditions. Any record containing a zero value is automatically identified and flagged for review.

Resolution: Users are required to either proceed with processing while retaining the zero CO_2-C entries or cancel the run, correct the source files, and rerun the module. Check and trace the output file and identify the Site IDs with zero (0) CO_2-C fluxes outputs and concentrations (ppm). The CO_2 concentrations over the hour sampling time period should be linear and the change of concentrations per time interval is significant. Check the factors affecting such concentrations: temperature, and other field/weather variables; possible sample vial leaks; interchanged vials sampled in a sampling time interval (t0, t1, t2, t3, t4). Re-analyze the samples in GC.

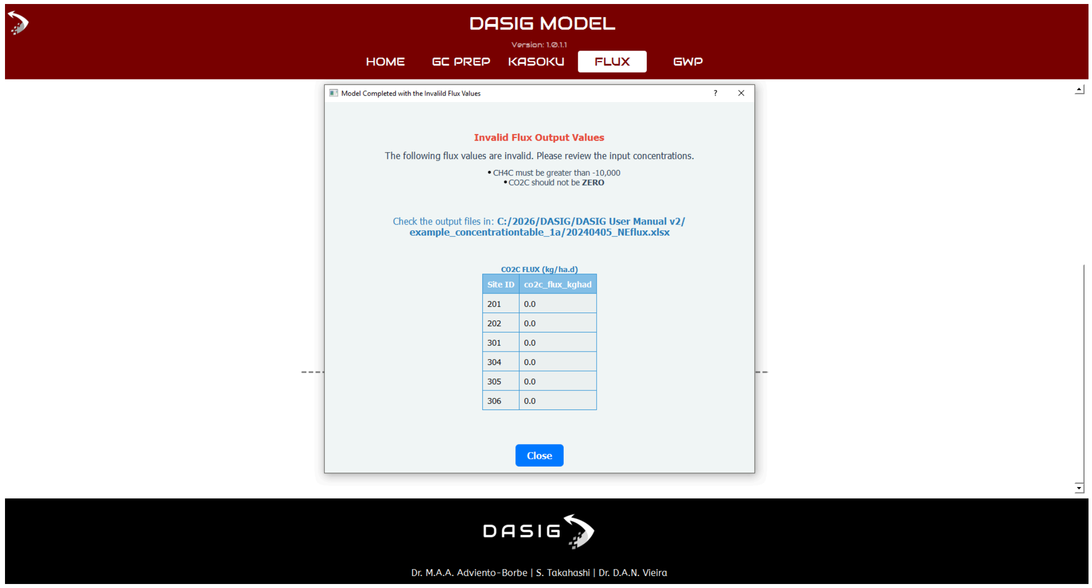


Figure 5.29. The FLUX module identifies zero CO_2-C outputs as '*Invalid Flux Output Values*' that require review of the input concentrations.

9. Glossary

Term	Definition
Concentration Table File	The Excel workbook with the data needed for the DASIG-FLUX module that contains the headspace input and ppm input.
HEADSPACE INPUT Sheet	The sheet in the Flux Input file that contains date of sampling (DATE), field ID (FIELD ID), site ID (SITE ID), block (BLOCK), treatment ID (TRT ID), headspace (HEADSPACE VOLUME (L)), and HEADSPACE AREA (m^2)
PPM INPUT Sheet	The sheet in the Flux Input file that contains the site ID (SITE ID), chamber temperatures (CHAMBER TEMP (°C)) per time interval (TIME (hour)) and the N_2O, CH_4, and CO_2 concentration values (CH_4 (ppm); N_2O (ppm); CO_2 (ppm)).
DATE	Date of gas sampling
FIELD ID	Experiment field identifier i.e. *NE* - North East experiment; *ST* - Stuttgart experiment
BLOCK	Replication of your samples under specific treatment

TRT ID	Treatment identifier based on the experimental design. For example, types of irrigation systems as treatment in different field location i.e. MIRI; Top Recirculating; Bottom Recirculating.
SITE ID	Individual chamber identification based on block and treatment numbers. i.e. 101-106 (1st replication of MIRI)
HEADSPACE VOLUME (L)	The volume of chamber headspace in liters (L).
HEADSPACE AREA (m^2)	The area of the chamber headspace in meter square .
CHAMBER TEMP (°C)	The chamber temperature measured during the sampling.
TIME (hour)	The sampling time interval in one hour sampling period.
CH_4 (ppm); N_2O (ppm); CO_2 (ppm)	The mass concentrations calculated using the peak areas from gas chromatograms. The data is derived from the KASOKU module.
Mass Concentration (MC, µg/L)	The mass per unit volume of gas at sampling temperature
Linear Flux	The slope of gas mass concentration over time.
Detection Limit (DL)	Detection limit is defined as the lowest concentration of a specific trace gas that can be reliably detected and statistically distinguished from the background noise or a blank sample.
R^2	The regression of concentration values (ppm) over time.
Daily Flux	Daily gas fluxes of N_2O, CO_2, and CH_4 as expressed in their elemental forms per hectare per day, based on the change of concentrations inside the chamber over time in a specific chamber's volume and the soil area it covers.
HMR Flux	The gas flux estimates generated using the Hutchinson–Mosier Regression (HMR) model.

HMR Ratio	The ratio of HMR flux / Linear flux

Chapter 6 - DASIG-GWP Module

1. Overview

The DASIG-GWP module represents the final stage of the DASIG analytical suite. It aggregates GHG fluxes across an entire crop cycle and converts them into CO_2-equivalent (CO_2-eq) values using IPCC AR reports Global Warming Potential factors over 100-yr and 20-yr time horizons for each chamber location. This enables standardized comparison of warming impacts across CH_4, CO_2, and N_2O under both 20-year and 100-year.

Input files exported from the DASIG-Flux model are automatically processed through grouping, interpolation, summarization, and GWP conversion to generate final emission metrics for treatment- and block-level analysis.

2. Quick Start

1. Create **Output Folder Name**
   Create a folder name for the results generated by the module.
2. Select **Select Working Folder**
   Choose and create an output directory where all DASIG-GWP generated files will be saved. All summary tables, plots, and reports generated by this model will be written to this folder.

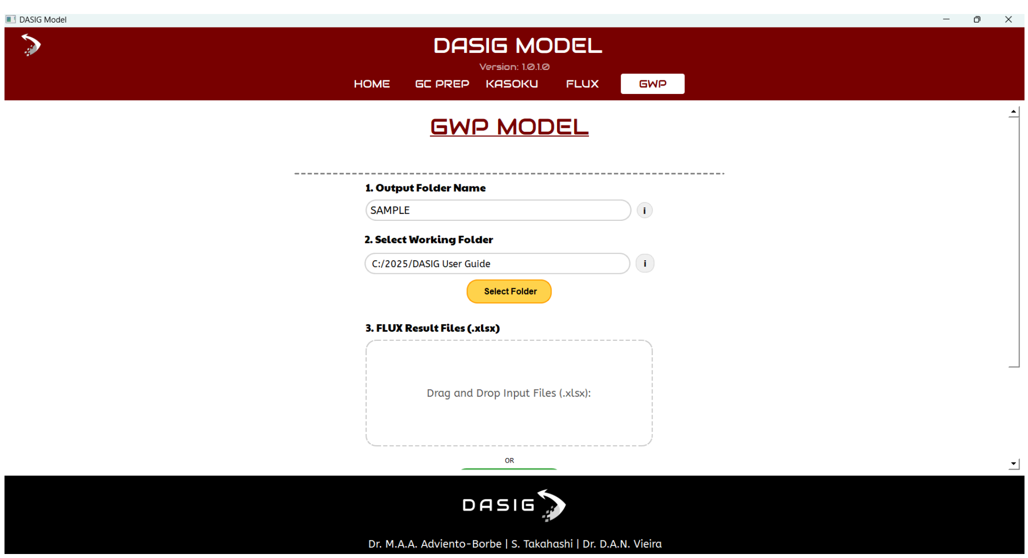


Figure 6.1. DASIG-GWP module interface for defining the output folder, selecting the working directory, and loading FLUX results files.

In Step 1, the user specifies the name of the output folder that will be created inside the working directory to store all GWP results. In Step 2, the user selects the working directory where the output folder will be generated.

3. Import Input Files
   Drag and drop, or use the *Open Files* button to import the workbooks generated by the DASIG FLUX Module (Daily Final Flux Report). Confirm that all required sheets and metadata fields are present before processing.

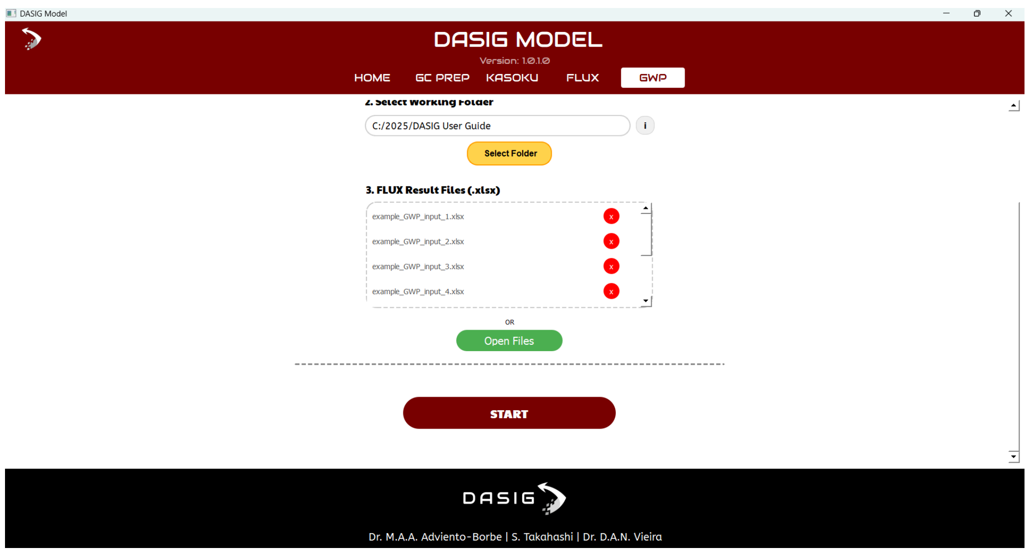


Figure 6.2. Multiple DASIG-FLUX result files loaded into the DASIG-GWP module for batch processing.

After selecting the working directory, users may upload DASIG-FLUX result files (.xlsx) into the GWP module. Each file appears in the upload panel as a separate entry, with an option to remove individual files if needed. When all desired files have been uploaded, the user proceeds by clicking **START**, and the GWP module processes each file sequentially to generate cumulative emissions and GWP summaries.

FINAL Flux Time Convert

DATE	FIELD ID	SITE ID	BLOCK	TRT ID	Flux (ug/m2.hr)			Flux (g/ha.d)			Flux (g/ha.d)			Flux (kg/ha.d)		
					CH4	N2O	CO2	CH4	N2O	CO2	CH4-C	N2O-N	CO2-C	CH4-C	N2O-N	CO2-C
2024-04-05	NE	101	1	MIRI	0	0	57613.53537	0	0	13827.24849	0	0	3771.06777	0	0	3.77106777
2024-04-05	NE	102	2	MIRI	0	8.084	52680.46065	0	1.94016	12643.31056	0	1.234647273	3448.175606	0	0.001234647	3.448175606
2024-04-05	NE	103	3	MIRI	0	0	56782.24477	0	0	13627.73874	0	0	3716.656021	0	0	3.716656021
2024-04-05	NE	104	4	MIRI	0	0	96532.64302	0	0	23167.83433	0	0	6318.500271	0	0	6.318500271
2024-04-05	NE	105	5	MIRI	0	10.87	130209.9985	0	2.6088	31250.39964	0	1.660145455	8522.836267	0	0.001660145	8.522836267
2024-04-05	NE	106	6	MIRI	0	-17.74	67440.71642	0	-4.2576	16185.77194	0	-2.709381818	4414.301438	0	-0.002709382	4.414301438
2024-04-05	NE	201	1	Top Recirculating	0	0	0	0	0	0	0	0	0	0	0	0
2024-04-05	NE	202	2	Top Recirculating	0	20.17	0	0	4.8408	0	0	3.080509091	0	0	0.003080509	0
2024-04-05	NE	203	3	Top Recirculating	0	0	57816.19842	0	0	13875.88762	0	0	3784.332988	0	0	3.784332988
2024-04-05	NE	204	4	Top Recirculating	0	18.87	48221.2902	0	4.5288	11573.10965	0	2.881963636	3156.302631	0	0.002881964	3.156302631
2024-04-05	NE	205	5	Top Recirculating	0	15.37	41727.493	0	3.6888	10014.59832	0	2.347418182	2731.254087	0	0.002347418	2.731254087
2024-04-05	NE	206	6	Top Recirculating	0	0		0	0		0	0		0	0	
2024-04-05	NE	301	1	Bottom Recirculating	0	-11.94	0	0	-2.8656	0	0	-1.823563636	0	0	-0.001823564	0
2024-04-05	NE	302	2	Bottom Recirculating	0	-9.112638235	30754.65898	0	-2.187033176	7381.118155	0	-1.391748385	2013.032224	0	-0.001391748	2.013032224
2024-04-05	NE	303	3	Bottom Recirculating	0	17.11	81121.20015	0	4.1064	19469.08803	0	2.613163636	5309.751282	0	0.002613164	5.309751282
2024-04-05	NE	304	4	Bottom Recirculating	0	0	0	0	0	0	0	0	0	0	0	0
2024-04-05	NE	305	5	Bottom Recirculating	0	11.86	0	0	2.8464	0	0	1.811345455	0	0	0.001811345	0
2024-04-05	NE	306	6	Bottom Recirculating	0	34.4770937	0	0	8.274502488	0	0	5.265592492	0	0	0.005265592	0

FLUX | FINAL FLUX | DAILY FINAL FLUX

Ready | Accessibility: Good to go

Figure 6.3. Sample daily soil-trace gas flux dataset formatted for input to the DASIG-GWP module.

This worksheet lists the finalized daily CH_4-C, N_2O-N, and CO_2-C fluxes for each sampling date, site, block, and treatment. Fluxes are provided in multiple unit conversions (e.g., µg $m^{-2}hr^{-1}$, g $ha^{-1}d^{-1}$, and kg $ha^{-1}d^{-1}$) to ensure compatibility with downstream calculations. These data are generated by the DASIG-FLUX module and serve as the standardized input for the cumulative emission for each chamber location and GWP computations in the DASIG-GWP module.

4. Run the DASIG-GWP module by clicking the **START** button (Figure 6.4). The model will automatically process all valid flux records and compute cumulative emissions and CO_2-equivalent values for each chamber location.
   a. UI Input Confirmation
      Review the loaded workbook within the user interface to ensure that all data fields and metadata have been correctly recognized.

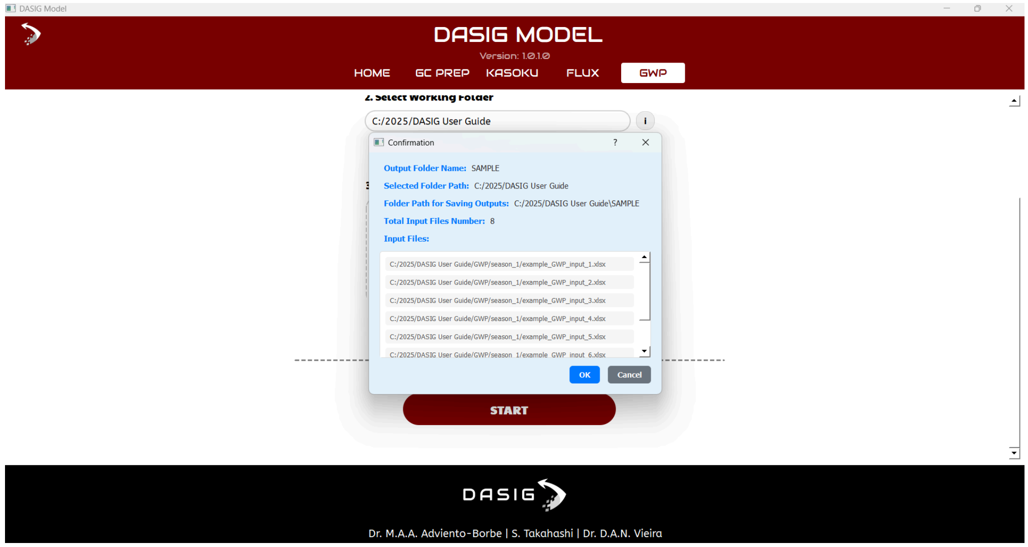


Figure 6.4. Confirmation dialog summarizing user selections prior to running the DASIG-GWP module.

Before execution, the DASIG-GWP module displays a confirmation window listing the output folder name, the selected working directory, the full path where the results will be saved, the total number of input files, and the file names to be processed. Users should review this information to verify that the correct folders and datasets have been selected. Processing begins once the user confirms by clicking **OK**.

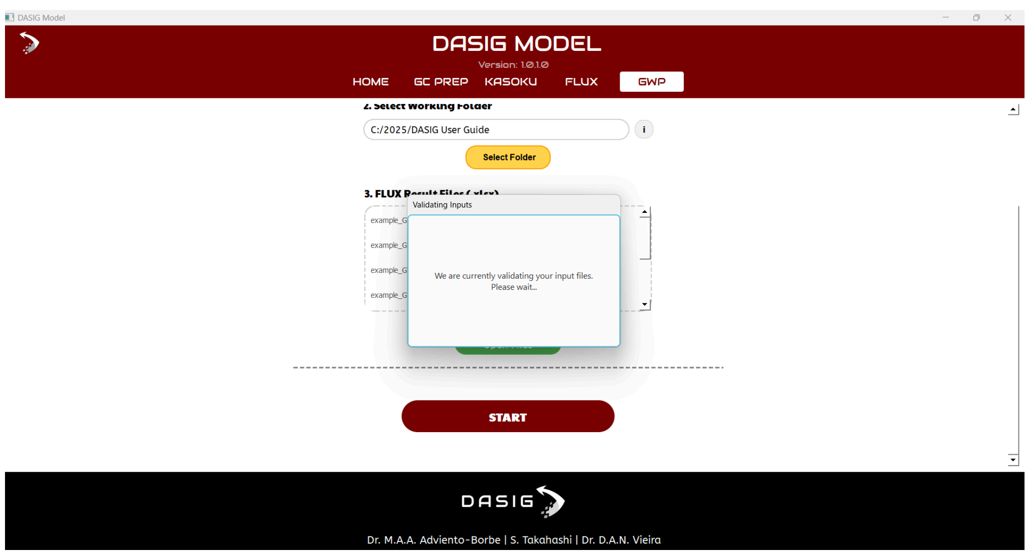


Figure 6.5. Input-file validation process in the DASIG-GWP module.

After the user confirms the selected folders and input files, the DASIG-GWP module performs an automated validation check. During this step, the software verifies that each uploaded file contains required worksheets, column headers, and data structure produced by the DASIG-Flux module. A progress window is displayed while validation is underway.

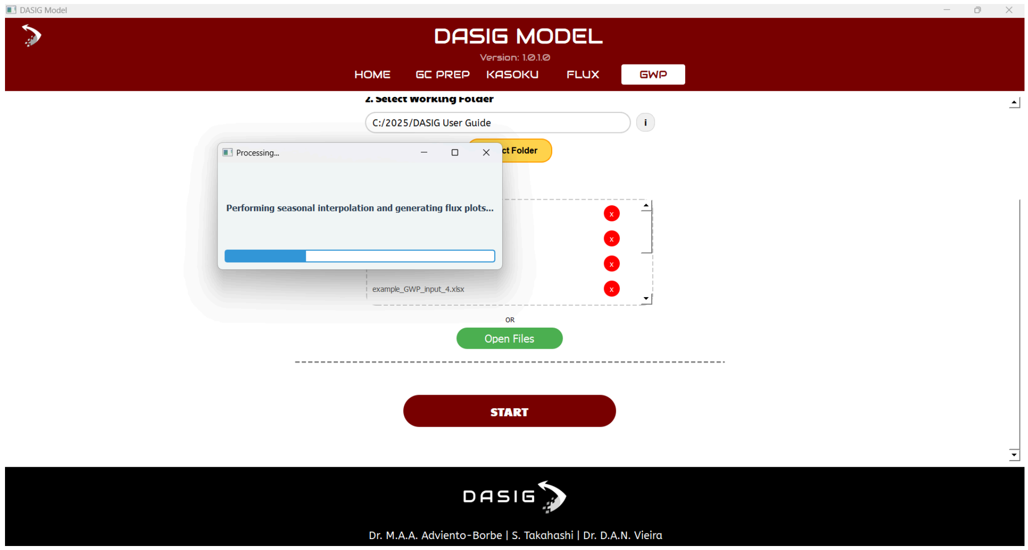


Figure 6.6. DASIG-GWP module processing seasonal flux data and generating diagnostic plots.

Once validation is complete and execution is confirmed, the DASIG-GWP module performs daily interpolation of CH_4-C, N_2O-N, and CO_2-C fluxes across the measurement period. During this stage, the software also generates time-series and cumulative-flux plots and computes seasonal emission totals and GWP metrics. A progress window is displayed while processing is underway.

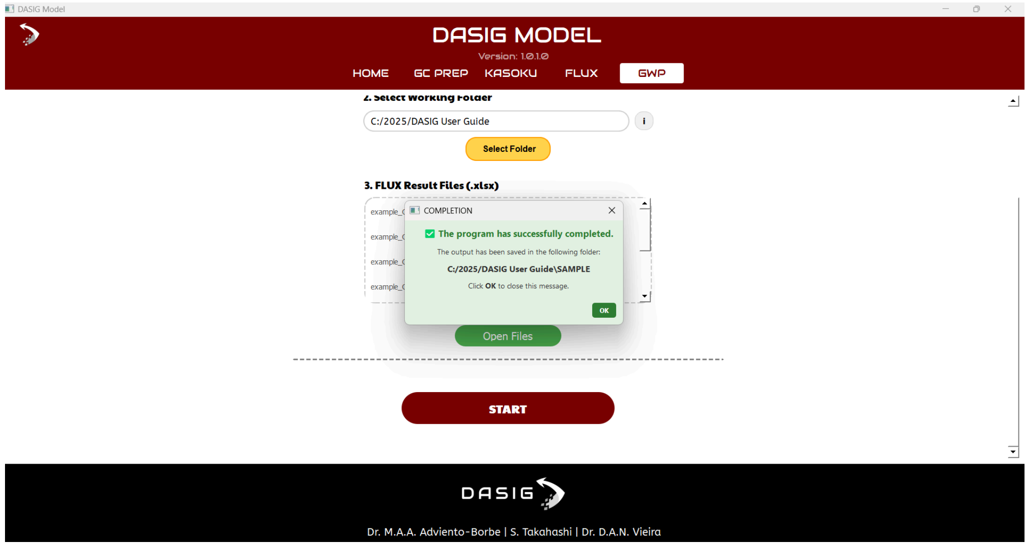


Figure 6.7. Completion message displayed after successful execution of the DASIG-GWP module.

When all selected FLUX result files have been processed, the DASIG-GWP module displays a completion dialog confirming that the program finished successfully. The message also provides the file path to the output folder created within the selected working directory. Users may close the dialog and navigate to this folder to view the generated emission summaries, GWP tables, and diagnostic plots.

5. Export Outputs
   All computed metrics are saved to the designated output folder, including:
   - Per-block and per-treatment emission tables with graphical plots
   - TRT_SUMMARY.xlsx as the final consolidated report

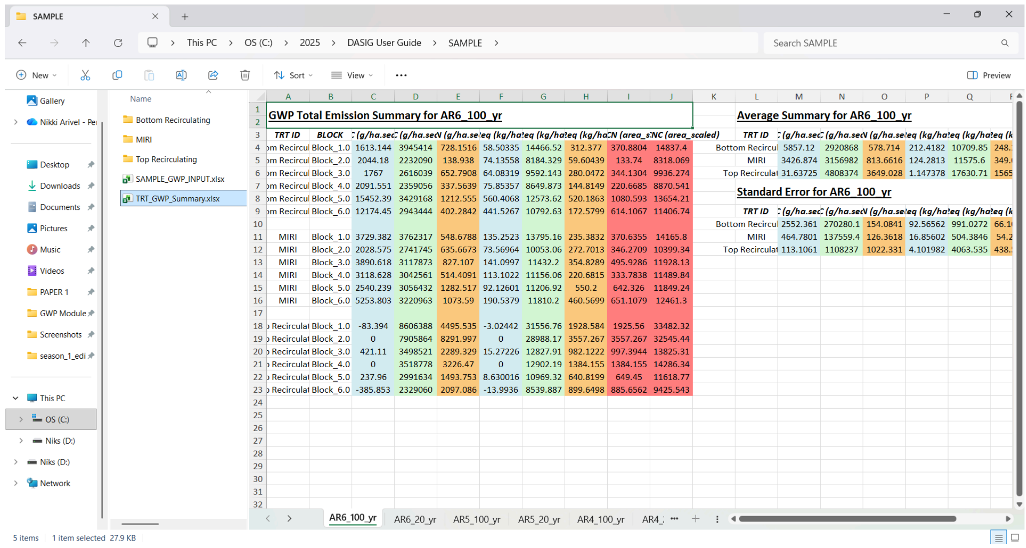


Figure 6.8. Output structure and treatment-level GWP summary workbook generated by the DASIG-GWP module.

For each treatment, the DASIG-GWP module creates a separate results folder containing the processed flux tables, interpolation plots, and seasonal cumulative emission outputs. In addition, a consolidated workbook (TRT_GWP_Summary.xlsx) is produced at the working-folder level. This workbook contains multiple worksheets corresponding to each selected IPCC assessment report and time horizon. Within each worksheet, replicate-level cumulative emissions and GWP values are reported on an area basis, along with the treatment-level averages and standard errors. These summaries support comparison of mean GWP outcomes among treatments, while standard error values indicate variability across replicates.

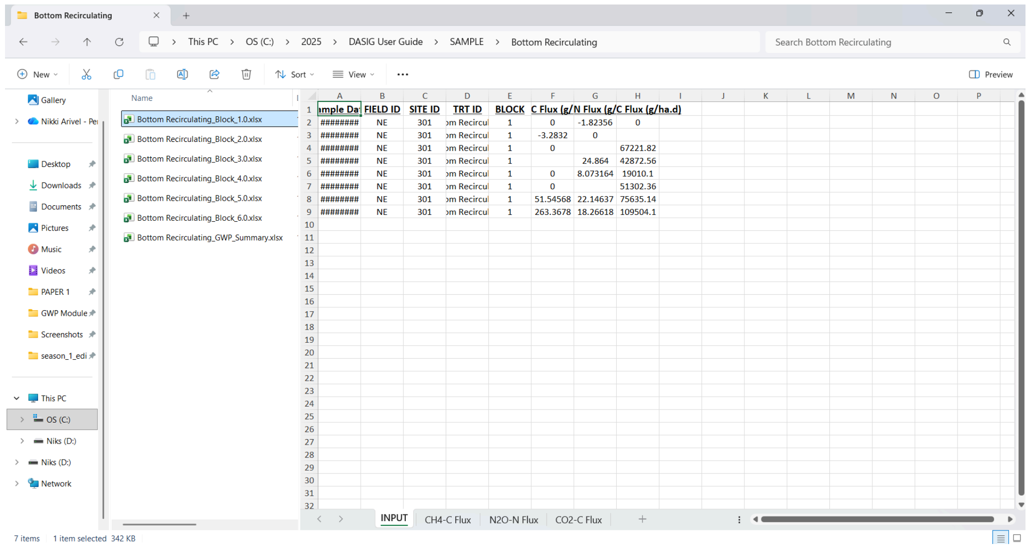


Figure 6.9. Example of treatment-level output folder generated by the DASIG-GWP module.

For each treatment, the DASIG-GWP module creates a dedicated results folder. Within this folder, one workbook is produced for every replicate or block. Each workbook contains multiple worksheets, including the original input flux data and the interpolation and cumulative CH_4-C, N_2O-N, and CO_2-C flux tables for the corresponding replicate. A separate treatment-level summary workbook is also generated to consolidate seasonal emission and GWP results across replicates for that treatment.

3. Input Specification

- The DASIG-GWP module requires Excel workbooks generated directly from the DASIG-FLUX module. These files contain the processed and quality-controlled daily flux estimates for each greenhouse gas and form the sole data source for GWP calculations. Only outputs from DASIG-FLUX should be used, as the GWP module assumes consistent formatting, variable naming, and unit structure.
  Each workbook must include the following core elements (see Figure 6.9):
    - Daily fluxes for CH_4-C, N_2O-N, and CO_2-C expressed on an area- and time-standardized basis
    - Sampling date corresponding to the day the flux was measured or interpolated
    - Treatment identifier (TRT ID)
    - Replication or block identifier

    - Site or field identifier (if applicable)
- Because cumulative seasonal emissions are obtained by integrating daily fluxes over time, only finalized values are accepted by the GWP module. Raw chamber readings or partially processed values are not supported.
- File and Sheet Requirements
    - Each treatment (or treatment-block combination, depending on user setup) must be supplied as a separate Excel workbook. The GWP module automatically scans each workbook for the required sheets and variables. Missing, blank, or non-numeric entries in the greenhouse-gas flux fields will trigger a validation message requesting user confirmation before proceeding.
- Consistency Requirement
    - All treatment files used in a single GWP run must cover the same date range, and contain at least two daily records to allow correct temporal integration.

4. Tips to Optimal Procedure

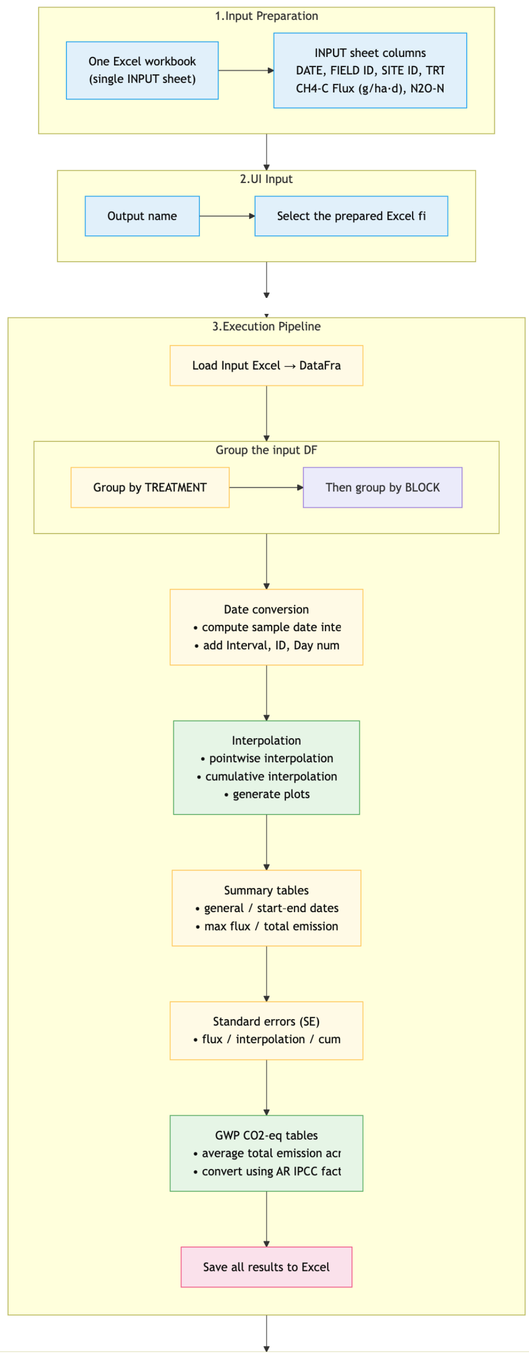
To ensure reliable GWP estimation, users are encouraged to review and prepare DASIG-FLUX outputs prior to running the GWP module:

- Confirm that all DASIG-FLUX outputs have passed quality-assurance screening.
  This includes review of detection-limit flags, removal or correction of abnormal recordings, and verification that gap-filling or interpolation (where applied) has been completed.
- Check sampling dates for completeness and correct formatting.
  Dates must be stored in valid date format to allow correct temporal integration of fluxes.
- Inspect CO_2-C flux values for unintended zero entries.
  True zero CO_2 flux is highly unlikely in vented chamber systems and may indicate missing data, formatting errors, or failed import. Unintended zeros can bias seasonal cumulative totals and GWP estimates.
- Ensure that treatment identifiers and block/replication labels are consistent across files.
  Inconsistent naming prevents correct grouping of emissions during GWP aggregation.
- Verify that units match the DASIG-FLUX output specification.
  Fluxes should be expressed on a daily, area-normalized basis (e.g., g ha^{-1} d^{-1} or kg ha^{-1} d^{-1}, depending on the gas and output sheet).
- Avoid editing DASIG-FLUX workbooks manually unless necessary.

Manual changes may alter formulas, remove metadata, or introduce hidden formatting errors that trigger validation warnings.

- Retain at least two sampling dates per treatment or block.
  Single-day flux records cannot be integrated over time and will not be processed.

5. Model Processing Flow



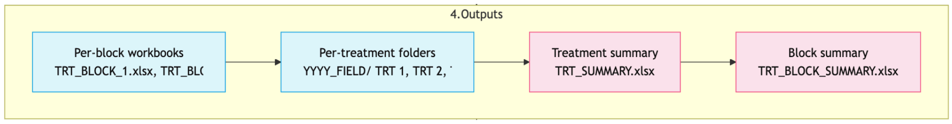


Figure 6.10. Flow diagram representing the core processing phases.

6. Quality Assurance / Quality Control (QA/QC)

- Before running the DASIG-GWP module, ensure that all input workbooks generated from the DASIG-FLUX module contain valid and complete flux data. The following checks are recommended:
    - Verify that CH_4, N_2O, and CO_2 flux fields contain numeric values only (no blanks, symbols, or text entries).
    - Confirm that no records are missing for required fields such as sampling date, treatment ID, site ID, and block ID.
    - Check that CO_2 flux values are not reported as zero, as true zero CO_2 exchange is physically unrealistic for vented chamber systems and may bias cumulative emission and GWP estimates.
    - Ensure detection-limit and data-quality screening has already been performed in the DASIG-FLUX module.

  Note: If inconsistencies or invalid entries are detected during processing, the GWP module automatically flags these cases in the warning prompts and output logs, allowing users to correct input files prior to rerunning the analysis.

7. Output Interpretation

- The DASIG-GWP module summarizes seasonal or period-based greenhouse-gas emissions on an area-scaled basis and expresses them as both mass units and CO_2-equivalent (CO_2-eq) units using IPCC GWP factors. Output tables include the following information:
    - CH_4-C, N_2O-N, and CO_2-C emissions
      These columns report the cumulative mass of each gas emitted over the selected period. Values are aggregated from daily measured and interpolated fluxes produced in the DASIG-FLUX module.
    - CH_4_CO_2eq and N_2O_CO_2eq
      These columns convert cumulative CH_4 and N_2O emissions into CO_2-equivalent units using the IPCC assessment report and time horizon. These metrics allow direct comparison of gases with different warming intensities.

- CO_2_CO_2eq
  CO_2 emissions are already expressed in CO_2-equivalent units; therefore, the numerical value is equal to the cumulative CO_2-C emission after appropriate conversion.
- GWP_CN (CH_4 + N_2O)
  This value represents the combined global-warming impact from CH_4 and N_2O only. It is useful when CO_2 emissions are accounted for separately or when comparing only non-CO_2 gases.
- GWP_CNC (CH_4 + N_2O + CO_2)
  This value represents the total GWP from all three gases combined over the selected period.
- Interpreting Treatment-Level Averages
  The average summary table presents the mean cumulative emissions and GWP values for each treatment. These values are calculated by averaging all replications within the same treatment and represent the typical seasonal emission level for that treatment. Users may use this table to compare overall greenhouse-gas performance among treatments on a consistent CO_2-equivalent basis. Higher values indicate greater seasonal emissions or warming impact for that gas.

- General guidance for interpretation
  - Higher GWP values indicate greater warming impact over the reporting period and can be compared across treatments, locations, or years, provided the same units and GWP horizon are used.
  - CH_4 and N_2O differ in warming intensity. Even small mass emissions of N_2O may contribute substantially to GWP because N_2O has a much larger CO_2-equivalent factor than CH_4 or CO_2.
  - Management practices may shift the balance between gases. For example, practices that reduce CH_4 emissions may influence N_2O emissions, and vice-versa. GWP metrics allow these trade-offs to be evaluated on a common scale.
  - Uncertainty and variability should be considered. The standard error columns indicate the variability of results among replications within each treatment. Users should interpret the differences among treatments in the context of this variability rather than relying on mean values alone.

- Recommended reporting practice

When presenting GWP results, users are encouraged to:

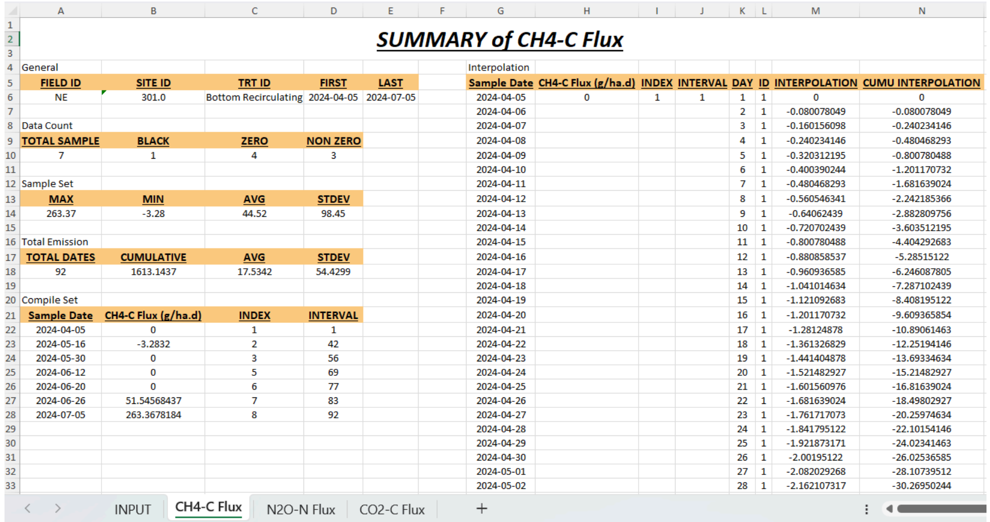
- Report the IPCC assessment report and time horizon using current conversions.
- State the spatial and temporal scale (e.g., per ha, per season)
- Clearly distinguish between GWP from CH_4+N_2O and GWP including CO_2, where relevant.
- When comparing treatments, users should ensure that:
    - The same IPCC report and time horizon are selected;
    - Emissions are expressed for the same time period and land area;
    - And the replication structure is comparable.
- Two different totals are generated. Users may report one or both depending on research or reporting objectives.

Sample Date	FIELD ID	SITE ID	TRT ID	BLOCK	CH4-C Flux (g/ha.d)	N2O-N Flux (g/ha.d)	CO2-C Flux (g/ha.d)
2024-04-05 0:00:00	NE	301	Bottom Recirculating	1	0	-1.823563636	0
2024-05-16 0:00:00	NE	301	Bottom Recirculating	1	-3.2832	0	
2024-05-30 0:00:00	NE	301	Bottom Recirculating	1	0		67221.81818
2024-06-05 0:00:00	NE	301	Bottom Recirculating	1		24.864	42872.55792
2024-06-12 0:00:00	NE	301	Bottom Recirculating	1	0	8.073163636	19010.09652
2024-06-20 0:00:00	NE	301	Bottom Recirculating	1	0		51302.36004
2024-06-26 0:00:00	NE	301	Bottom Recirculating	1	51.54568437	22.14637483	75635.14068
2024-07-05 0:00:00	NE	301	Bottom Recirculating	1	263.3678184	18.26618182	109504.1445

INPUT | CH4-C Flux | N2O-N Flux | CO2-C Flux

Figure 6.11. Example input dataset used by the DASIG-GWP module.

This worksheet contains the finalized daily soil trace-gas fluxes generated by the DASIG-FLUX module. Each record includes the sampling date, site and treatment identifiers, block number, and the corresponding CH_4-C, N_2O-N, and CO_2-C flux values expressed on an area basis (e.g., g $ha^{-1}d^{-1}$). These values are used as the baseline inputs for daily interpolation and cumulative seasonal emission calculations performed by the DASIG-GWP module.



SUMMARY of CH4-C Flux

General

FIELD ID	SITE ID	TRT ID	FIRST	LAST
NE	301.0	Bottom Recirculating	2024-04-05	2024-07-05

Data Count

TOTAL SAMPLE	BLACK	ZERO	NON ZERO
7	1	4	3

Sample Set

MAX	MIN	AVG	STDEV
263.37	-3.28	44.52	98.45

Total Emission

TOTAL DATES	CUMULATIVE	AVG	STDEV
92	1613.1437	17.5342	54.4299

Compile Set

Sample Date	CH4-C Flux (g/ha.d)	INDEX	INTERVAL
2024-04-05	0	1	1
2024-05-16	-3.2832	2	42
2024-05-30	0	3	56
2024-06-12	0	5	69
2024-06-20	0	6	77
2024-06-26	51.54568437	7	83
2024-07-05	263.3678184	8	92

Interpolation

Sample Date	CH4-C Flux (g/ha.d)	INDEX	INTERVAL	DAY	ID	INTERPOLATION	CUMU INTERPOLATION
2024-04-05	0	1	1	1	1	0	0
2024-04-06				2	1	-0.080078049	-0.080078049
2024-04-07				3	1	-0.160156098	-0.240234146
2024-04-08				4	1	-0.240234146	-0.480468293
2024-04-09				5	1	-0.320312195	-0.800780488
2024-04-10				6	1	-0.400390244	-1.201170732
2024-04-11				7	1	-0.480468293	-1.681639024
2024-04-12				8	1	-0.560546341	-2.242185366
2024-04-13				9	1	-0.64062439	-2.882809756
2024-04-14				10	1	-0.720702439	-3.603512195
2024-04-15				11	1	-0.800780488	-4.404292683
2024-04-16				12	1	-0.880858537	-5.28515122
2024-04-17				13	1	-0.960936585	-6.246087805
2024-04-18				14	1	-1.041014634	-7.287102439
2024-04-19				15	1	-1.121092683	-8.408195122
2024-04-20				16	1	-1.201170732	-9.609365854
2024-04-21				17	1	-1.28124878	-10.89061463
2024-04-22				18	1	-1.361326829	-12.25194146
2024-04-23				19	1	-1.441404878	-13.69334634
2024-04-24				20	1	-1.521482927	-15.21482927
2024-04-25				21	1	-1.601560976	-16.81639024
2024-04-26				22	1	-1.681639024	-18.49802927
2024-04-27				23	1	-1.761717073	-20.25974634
2024-04-28				24	1	-1.841795122	-22.10154146
2024-04-29				25	1	-1.921873171	-24.02341463
2024-04-30				26	1	-2.00195122	-26.02536585
2024-05-01				27	1	-2.082029268	-28.10739512
2024-05-02				28	1	-2.162107317	-30.26950244

INPUT | CH4-C Flux | N2O-N Flux | CO2-C Flux

Figure 6.12. Example replicate-level seasonal flux summary and interpolation worksheet generated by the DASIG-GWP module.

Each treatment-replicate workbook contains gas-specific worksheets summarizing measured fluxes and interpolated daily values across the monitoring period. The worksheet shows general site and sampling information, basic descriptive statistics for the measured sample set, cumulative seasonal emissions, and the interpolation series used to construct daily and cumulative flux estimates for CH_4-C. Corresponding worksheets are also generated for N_2O-N and CO_2-C, following the same structure and reporting format.

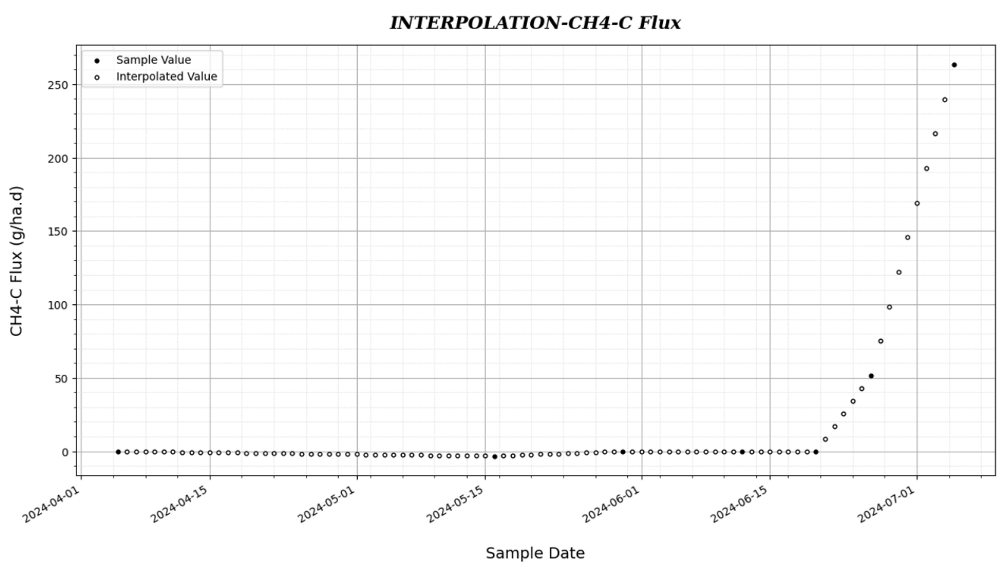


Figure 6.14. Example of seasonal flux interpolation plot generated by the DASIG-GWP module (CH_4-C shown as a representative gas).

For each treatment, the DASIG-GWP module produces an interpolation plot showing measured flux observations (filled circles) and the corresponding interpolated daily flux values (unfilled circles) across the monitoring period. These interpolated values are used to estimate cumulative seasonal emissions. Similar interpolation plots are also generated for N_2O-N and CO_2-C using the same graphical format.

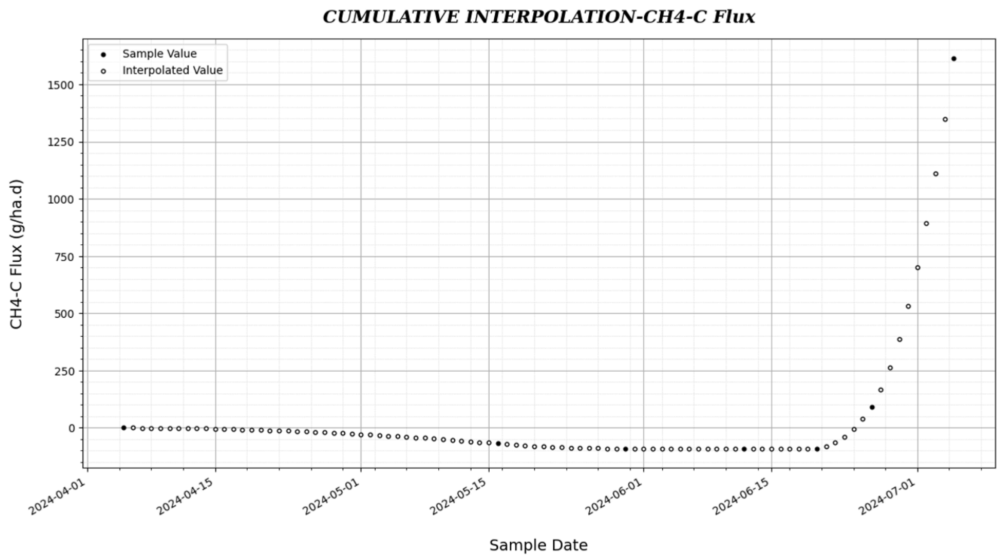
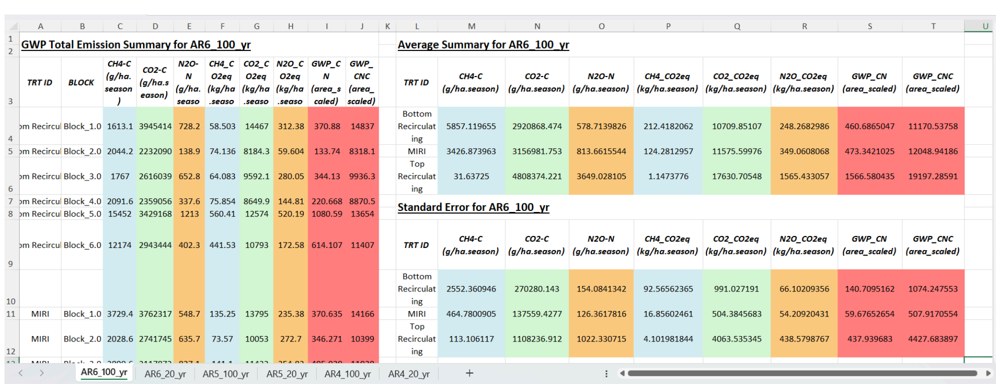


Figure 6.15. Example of cumulative seasonal flux interpolation plot generated by the DASIG-GWP module (CH_4-C shown as a representative gas).

For each treatment. The DASIG-GWP module also generates a cumulative interpolation plot in which the interpolated daily flux values are summed across the monitoring period. Measured observations (filled circles) and interpolated cumulative values (unfilled circles) are displayed together to illustrate how seasonal emissions build over time. Equivalent cumulative plots are produced for N_2O-N and CO_2-C using the same plotting format.



GWP Total Emission Summary for AR6_100_yr

TRT ID	BLOCK	CH4-C (g/ha.season)	CO2-C (g/ha.season)	N2O-N (g/ha.seaso	CH4_CO2eq (kg/ha.seaso	CO2_CO2eq (kg/ha.seaso	N2O_CO2eq (kg/ha.seaso	GWP_CN (area_scaled)	GWP_CNC (area_scaled)
om Recircul	Block_1.0	1613.1	3945414	728.2	58.503	14467	312.38	370.88	14837
om Recircul	Block_2.0	2044.2	2232090	138.9	74.136	8184.3	59.604	133.74	8318.1
om Recircul	Block_3.0	1767	2616039	652.8	64.083	9592.1	280.05	344.13	9936.3
om Recircul	Block_4.0	2091.6	2359056	337.6	75.854	8649.9	144.81	220.668	8870.5
om Recircul	Block_5.0	15452	3429168	1213	560.41	12574	520.19	1080.59	13654
om Recircul	Block_6.0	12174	2943444	402.3	441.53	10793	172.58	614.107	11407
MIRI	Block_1.0	3729.4	3762317	548.7	135.25	13795	235.38	370.635	14166
MIRI	Block_2.0	2028.6	2741745	635.7	73.57	10053	272.7	346.271	10399

Average Summary for AR6_100_yr

TRT ID	CH4-C (g/ha.season)	CO2-C (g/ha.season)	N2O-N (g/ha.season)	CH4_CO2eq (kg/ha.season)	CO2_CO2eq (kg/ha.season)	N2O_CO2eq (kg/ha.season)	GWP_CN (area_scaled)	GWP_CNC (area_scaled)
Bottom Recirculating	5857.119655	2920868.474	578.7139826	212.4182062	10709.85107	248.2682986	460.6865047	11170.53758
MIRI	3426.873963	3156981.753	813.6615544	124.2812957	11575.59976	349.0608068	473.3421025	12048.94186
Top Recirculating	31.63725	4808374.221	3649.028105	1.1473776	17630.70548	1565.433057	1566.580435	19197.28591

Standard Error for AR6_100_yr

TRT ID	CH4-C (g/ha.season)	CO2-C (g/ha.season)	N2O-N (g/ha.season)	CH4_CO2eq (kg/ha.season)	CO2_CO2eq (kg/ha.season)	N2O_CO2eq (kg/ha.season)	GWP_CN (area_scaled)	GWP_CNC (area_scaled)
Bottom Recirculating	2552.360946	270280.143	154.0841342	92.56562365	991.027191	66.10209356	140.7095162	1074.247553
MIRI	464.7800905	137559.4277	126.3617816	16.85602461	504.3845683	54.20920431	59.67652654	507.9170554
Top Recirculating	113.106117	1108236.912	1022.330715	4.101981844	4063.535345	438.5798767	437.939683	4427.683897

AR6_100_yr | AR6_20_yr | AR5_100_yr | AR5_20_yr | AR4_100_yr | AR4_20_yr

Figure 6.16. Example treatment-level GWP summary worksheet generated by the DASIG-GWP module (AR6-100 yr shown).

The consolidated summary workbook (TRT_GWP_Summary.xlsx) contains separate worksheets for each IPCC assessment report and time horizon. Each worksheet reports seasonal cumulative emissions of CH_4-C, N_2O-N, and CO_2-C on an area basis, together with their corresponding CO_2-equivalent values and combined GWP metrics. Replicate-level totals are listed for each treatment, along with treatment-level averages and standard errors. The worksheet shown corresponds to the AR6-100 yr GWP scenario; the remaining worksheets follow the same format.

8. Troubleshooting

Issue:	Fewer than two FLUX result files selected
Impact:	The DASIG-GWP module cannot organize results by treatment and replicate or generate treatment-level summary tables. Processing is halted and an input-error message is displayed.
Resolution:	Add at least one additional DASIG-FLUX result file and restart the GWP module. A minimum of two files is required to support treatment grouping and summary output generation.

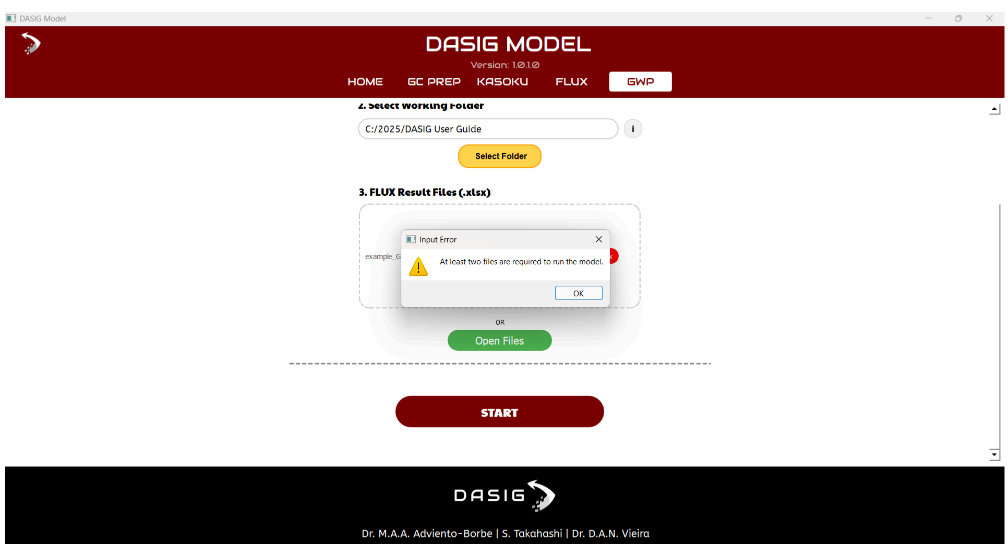


Figure 6.17. Input-validation warning displayed when insufficient FLUX files are provided.

Issue:	Zero CO_2-C flux values detected
Impact:	CO_2-C flux values equal to zero are physically unrealistic under

field conditions using vented chambers and may indicate missing data, formatting errors, or failed data processing. These values can bias cumulative emissions and GWP calculations if not corrected.

Resolution: Review the listed records in the warning dialog and verify the corresponding source files. Users may either correct the input data and rerun the model or proceed with the flagged values if they are known to be valid.

Note: Because CO_2 is continuously produced by soil and plant respiration, a true CO_2-C flux of exactly zero is highly unlikely under field conditions. Therefore, zero CO_2-C flux values are flagged as potentially invalid and users are advised to verify their source data.

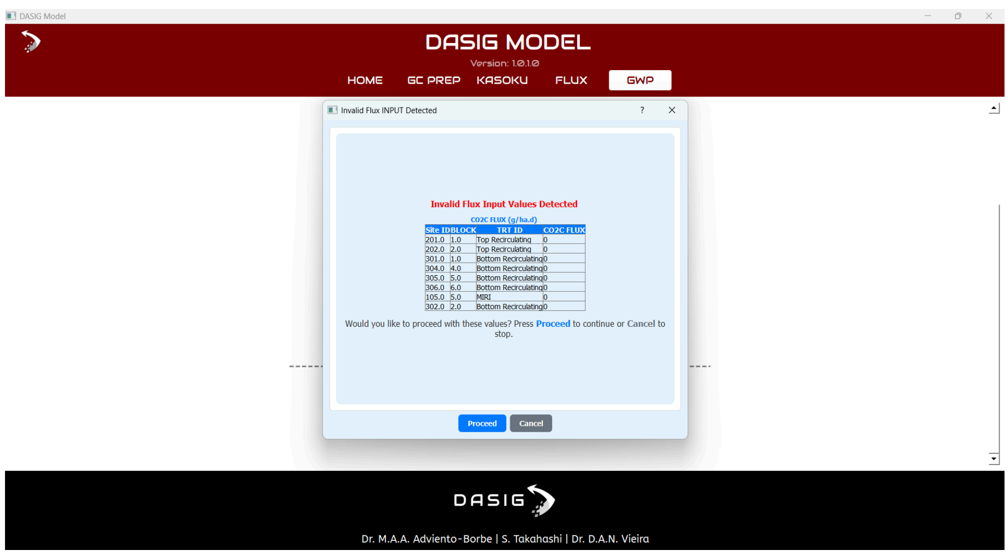


Figure 6.18. Warning dialog displayed when zero CO_2-C flux values are detected in the input data.

Issue: Empty or unreadable FLUX result file

Impact: The GWP module cannot process files that contain no valid data records. Execution is stopped to prevent generation of incomplete or invalid output.

Resolution: Replace the empty file with a valid DASIG-FLUX result workbook and rerun the GWP module.

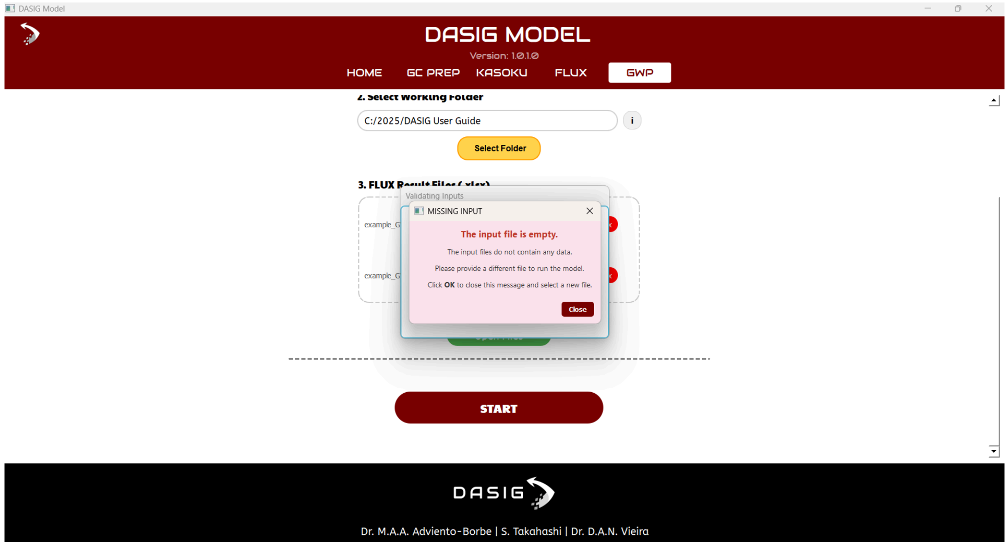


Figure 6.19. Missing-input warning displayed when an uploaded FLUX file contains no data.

Issue:	Non-numeric values in flux columns
Impact:	Text entries, blanks, or invalid characters in the CH_4-C, N_2O-N, or CO_2-C columns prevent numerical integration and GWP calculations. Affected files are flagged during validation.
Resolution:	Open the flagged FLUX result files and correct all non-numeric entries. Then reload the corrected files into the DASIG-GWP module and rerun the analysis.

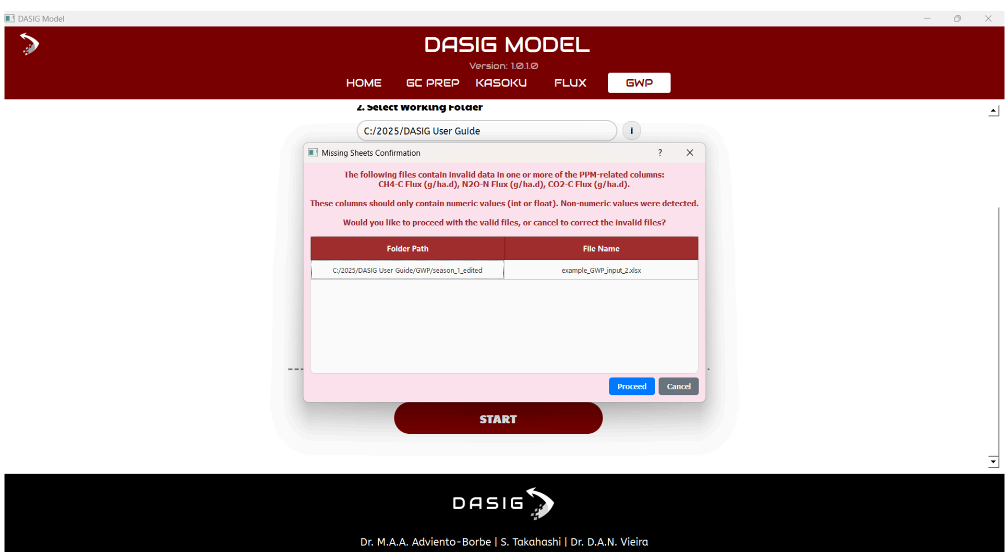


Figure 6.20. Invalid numeric-data warning for PPM-related flux columns during input validation.

9. Glossary

Term	Definition
Global Warming Potential (GWP)	A metric that describes the cumulative warming effect of a greenhouse gas relative to CO_2 over a specified time period (e.g., 20 or 100 years). GWP integrates both the gas's radiative efficiency and atmospheric lifetime.
CO_2-equivalent (CO_2-eq)	The amount of CO_2 that would produce the same cumulative radiative forcing as a given quantity of non-CO_2 gas (e.g., CH_4 or N_2O) over a specified time horizon. CO_2-eq allows emissions of different gases to be compared on a common scale.
IPCC AR6 (2021) Global Warming Potential factors	Standardized conversion factors published by the Intergovernmental Panel on Climate Change (IPCC) in the Sixth Assessment Report (AR6). These factors express the warming impact of a greenhouse gas relative to CO_2 over a defined time horizon (e.g., 20-yr or 100-yr).
Flux (or Gas Flux)	The rate at which a gas is emitted from or absorbed by the soil surface, expressed per unit area and time (e.g., g ha^{-1} d^{-1}).
Cumulative Emissions	The total quantity of gas emitted over a monitoring period, calculated by integrating (summing) daily or interpolated gas fluxes across time.
Interpolation	A method used to estimate gas flux values on unsampled days based on neighboring measured values. This allows continuous emission time-series to be constructed.

Appendix A - Glossary

Chapter No.	Term	Description
2	GC Metasolver	An Excel worksheet used to prepare and generate the GC run sequence script prior to GC analysis. It is part of the DASIG model resources and contains fields for entering gas sampling date, site ID, batch information, and gas sample IDs to produce a randomized analytical sequence.
2	Preparation Tab	A main tab within the GC Prep Datasheet file where users input required run parameters such as the sampling date, Site ID, batch number, and sample list.This serves as the starting point for creating the GC run sequence.
2	Batch Tab	A supplementary tab within the GC Prep Datasheet file that is to generate and display the finalized batch run order that GC instrument uses to sequentially analyze gas sample, derived from the input and randomization performed in the Preparation tab.
2	SITE ID Order tab	A tab within the GC metasolver file where users input the SITE IDs, TIME IDs, and the distribution of ambient field gas samples (AMB) to specific sets of SITE IDs for the time interval 0 min.
2	DATE	Date of gas sampling (mm/dd/yyyy).
2	SITE	The field experimental identification.
2	No (NO)	The fixed sequential number of gas samples.
2	SITE ID (Site ID)	The individual identification based on block and treatment numbers.
2	Time (TIME)	the time interval of gas sampling in minutes (e.g., 0, 15, 30, 45, 60).
2	TIME ID	The identification of the time interval during gas sampling (e.g., t0, t1, t2, t3, t4)

2	Order (ORDER)	The identification number that is specific to the sample and gets randomized after sorting the RAND() column.
2	RAND() formula =RAND()	An Excel random-number generating function used in the Preparation tab to assign a random value to each gas sample entry. The generated random numbers are used to randomize the sample run order, minimizing measurement bias and improving the reliability of the GC analysis.
2	EVENT	The concatenated DATE and SITE ID (yyyy.mm.ddSITEID).
2	SET	The identifier for calibration standard and sample gas.
2	CODE	The running number of gas standards and samples.
2	SAMPLE ID	The concatenated ID contains the sampling EVENT, SITE ID, TIME and ORDER.
2	formula =RAND()	An Excel random-number generating function used in the Preparation tab to assign a random value to each gas sample entry. The generated random numbers are used to randomize the sample run order, minimizing measurement bias and improving the reliability of the GC analysis.
3	Shimadzu GC 2014/2030	Gas chromatograph model manufactured by Shimadzu, supported as an input source for DASIG-GC-PREP preprocessing.
3	Shimadzu LabSolutions	Shimadzu’s chromatography data software system is used to manage gas analyses, collect data, integrate peaks and heights of chromatograms, and generate GC analysis reports and raw output files.
3	raw .txt output file	Text-based GC report files exported from Shimadzu LabSolutions, used as input files for the DASIG-GC-PREP module.
3	Peak Area Tables	Structured tabular datasets generated from raw GC outputs generated by GC-PREP module, containing retention times and peak areas for target gases. This is the input file

		for the KASOKU module.
3	Clean Table Step	A preprocessing step in DASIG-GC-PREP that removes irrelevant entries and standardizes data structure prior to splitting.
3	Split Table Step	A preprocessing step in DASIG-GC-PREP that divides cleaned datasets into logical segments for individual report generation.
3	DASIG Analytical Data Standards	Internal data standards that define formatting, structure, and quality requirements for analytical data within the DASIG model.
4	Batch (worksheet)	Summary of complete randomized sampling event including standard gases.
4	CH_4 Peak Area	Peak area for methane.
4	CH_4 Retention Time	Retention time for methane.
4	CO_2 Peak Area	Peak area for carbon dioxide.
4	CO_2 Retention Time	Retention time for carbon dioxide.
4	Coefficient of Variance (CV)	Statistical measure that expresses the amount of variability in each standard gas relative to its mean.
4	Coefficient of Determination (R^2)	Indicates the linearity and reliability for quantifying standard gas from peak area data.
4	Combination	List of peak area values used for analysis

4	Count	Number of samples included in QA/QC statistical metrics calculation.
4	CV	Coefficient of variation ($STDEV \div MEAN$) for the selected peak area combination.
4	Date and Time	Timestamp of analysis.
4	Gas	Target analyte (CH_4, N_2O, CO_2).
4	MEAN	Average peak areas across the combination.
4	N_2O Peak Area	Peak areas for nitrous oxide.
4	N_2O Retention Time	Retention time for nitrous oxide
4	Outlier	Number of samples flagged as statistical outliers across the peak area combination.
4	Peak Area	Represents the integrated electrical response produced by a compound as it passes through the detector.
4	Peak Table File (.xlsx)	A tabulated summary of data obtained from gas chromatography analysis. It lists the area under each peak in the chromatogram, which corresponds to the quantity of CH_4, N_2O, and CO_2 detected in the standard and samples.
4	Preparation File (.xlsx)	An Excel document that records how each batch was prepared prior to injection into the gas chromatography (GC) instrument. The file contains three worksheets namely *Preparation*, *Batch*, and *SITE ID Order*. Each worksheet provides specific details necessary for accurate and traceable sample preparation.
4	Preparation (worksheet)	Used to randomize gas samples for each batch by applying the RAND function.
4	Retention Time	Elapsed time between a sample's injection into the GC instrument and the moment a

		specific compound reaches a detector. It represents how long the compound spends traveling through the chromatographic column.
4	Sample ID	Unique identifier for each sample.
4	SITE ID Order (worksheet)	Describes the ambient (AMB) gases distribution within the experimental site.
4	Standards	Calibration standard used (e.g., AMB, 10M, 1N100M1kC, 3N500M10kC).
4	STDEV	Standard deviation of the peak areas.
	Flux Input file	The Excel workbook with the data needed for the DASIG-FLUX module run.
5	HEADSPACE INPUT Sheet	The sheet in the Flux Input file that contains date of sampling (DATE), field ID (FIELD ID), site ID (SITE ID), block (BLOCK), treatment ID (TRT ID), headspace (HEADSPACE VOLUME (L)), and HEADSPACE AREA (m^2)
5	PPM INPUT Sheet	The sheet in the Flux Input file that contains the site ID (SITE ID), chamber temperatures (CHAMBER TEMP (°C)) per time interval (TIME (hour)) and the N_2O, CH_4, and CO_2 concentration values (CH_4 (ppm); N_2O (ppm); CO_2 (ppm)).
5	DATE	Date of gas sampling
5	FIELD ID	Experiment field identifier i.e. *NE* - North East experiment; *ST* - Stuttgart experiment
5	BLOCK	Replication of your samples under specific treatment
5	TRT ID	Treatment identifier based on the experimental design. For example, types of irrigation systems as treatment in different field location i.e. MIRI; Top Recirculating; Bottom Recirculating.
5	SITE ID	Individual chamber identification based on block and treatment numbers. I.e. 101-106 (1st replication of MIRI)

5	HEADSPACE VOLUME (L)	The volume of chamber headspace in liters (L).
5	HEADSPACE AREA (m^2)	The area of the chamber headspace, expressed in square meters.
5	CHAMBER TEMP (°C)	The chamber temperature measured during the sampling.
5	TIME (hour)	The sampling time interval in one hour sampling period.
5	CH_4 (ppm); N_2O (ppm); CO_2 (ppm)	The mass concentrations calculated using the peak areas from gas chromatograms. The data is derived from the KASOKU module.
5	Mass Concentration (MC, µg/L)	The mass per unit volume of gas at sampling temperature
5	Linear Flux	The slope of gas mass concentration over time.
5	Detection Limit (DL)	Detection limit is defined as the lowest concentration of a specific trace gas that can be reliably detected and statistically distinguished from the background noise or a blank sample.
5	R^2	The regression of concentration values (ppm) over time.
5	Daily Flux	Daily gas fluxes of N_2O, CO_2, and CH_4 as expressed in their elemental forms per hectare per day, based on the change of concentrations inside the chamber changed over time in a specific chamber's volume and the soil area it covers.
5	HMR Flux	The gas flux estimates generated using the Hutchinson–Mosier Regression (HMR) model.

5	HMR Ratio	The ratio of HMR flux / Linear flux
6	Global Warming Potential (GWP)	A metric that describes the cumulative warming effect of a greenhouse gas relative to CO_2 over a specified time period (e.g., 20 or 100 years). GWP integrates both the gas's radiative efficiency and atmospheric lifetime.
6	CO_2-equivalent (CO_2-eq)	The equivalent amount of CO_2 that would produce the same cumulative radiative forcing as a given quantity of non-CO_2 (e.g., CH_4 or N_2O) over a specified time horizon.
6	IPCC AR6 (2021) Global Warming Potential factors	Standardized conversion factors published by the Intergovernmental Panel on Climate Change (IPCC) in the Sixth Assessment Report (AR6). These factors express the warming impact of a non-CO_2 gas relative to CO_2 over a defined time horizon (e.g., 20-yr or 100-yr).
6	Flux (or Gas Flux)	The rate at which a gas is emitted from or absorbed by the soil surface, expressed per unit area and time (e.g., g ha^{-1} d^{-1}).
6	Cumulative Emissions	The total quantity of gas emitted over a monitoring period, calculated by integrating (summing) daily or interpolated gas fluxes across time.
6	Interpolation	A method used to estimate gas flux values on unsampled days based on neighboring measured values. This allows continuous emission time-series to be constructed.

Appendix B - Troubleshooting Guide

Chapter No.	Issue	Impact	Resolution

1	DASIG installer cannot be downloaded	Installation cannot proceed.	Some institutional or secured networks restrict executable (.exe) downloads. Use an alternative network if needed and select Keep or Keep anyway when prompted by the web browser.
1	Browser security warnings block the installer	The setup file is blocked or removed during download.	Web browsers commonly warn when downloading executable files. Follow the browser-specific prompt and select Keep or Keep anyway to retain the installer.
1	Installation is blocked on institutional or managed computers	DASIG cannot be installed due to system restrictions or insufficient permissions.	Install DASIG for the current user when possible. If installation is blocked, contact local IT support for assistance or temporary permissions. For federal computers, unblock the software (under PROPERTIES/GENERAL) before the installation.
1	Antivirus or security software prevents the installer from running	The installer downloads but does not launch or is immediately blocked.	Some security programs restrict applications downloaded from the internet. Check security software settings and allow or whitelist the DASIG installer or temporarily permit execution during installation.
2	Inconsistent column headers, SITE IDs in Preparation tab and SITE ID order tab, and tab names.	The DASIG-KASOKU module fails to execute.	Use the GC metasolver template provided for consistent names of columns and sheets. Check and verify the inputs are the same in all the GC metasolver workbook tabs.

2	Mismatch details or information of SAMPLE ID in the Batch tab.	The DASIG-KASOKU module fails to execute.	The information should match the DATE*SITE*SITE ID*TIME*ORDER i.e. 2024.04.12STUT. ST.*303*40*49 per sample.
2	Inconsistent ambient field gas samples distribution in SITE ID Order tab.	An error in sample identification, therefore the DASIG-KASOKU module fails to execute, or wrong outputs.	Verify the SITE IDs and TIME IDs based on the inputs in the Preparation tab and ambient field gas samples distribution.
3	GC report file cannot be imported	The GC-PREP module cannot proceed, and no peak tables are generated.	Confirm that the input file is a raw text (txt) report exported directly from Shimadzu LabSolutions (Models 2014 or 2030). Ensure required sections (e.g., Header, Configuration, Peak Table) are present and re-export the file if necessary.
3	One or more imported files appear incomplete or empty	Merged peak tables may be misaligned by date or sequence.	Use the Merge & Reorder Peaks step to manually reorder files by sampling date and time and verify the sequence in the preview pane before merging.
3	Unwanted rows appear in the merged peak table	Non-sample rows may propagate into exported Excel files and affect downstream analysis.	Use the Clean Table step to remove irrelevant rows and review selections carefully before finalizing.

3	Incorrect table splitting or missing split points	Multiple sampling dates or analytical batches may be combined incorrectly.	Apply the Split Table step when datasets contain multiple sampling dates and confirm split boundaries during the Final Review.
3	Exported Excel files do not match expected structure	Downstream modules (e.g., DASIG-KASOKU) may reject the files or produce errors.	During Final Review, verify that CH_4, N_2O, and CO_2 peak areas are populated correctly, sample identifiers are intact, and record counts match expectations.
3	Need to revise or repeat preprocessing steps	Users may be uncertain whether the entire workflow must be repeated.	Previously exported GC-PREP Excel files can be re-imported for additional cleaning, merging, or splitting without reloading the original LabSolutions reports.
4	File Assignment Error	The KASOKU module cannot extract retention times or peak area values for CH_4, N_2O, and CO_2, preventing regression and quantification and halting the workflow.	Load the Peak Areas Table into the Peaks Input field and the Preparation File into the Prep Input field. Verify that the Peak Areas Table contains all required columns with correct naming and formatting, then re-upload both files.
4	Missing Retention Time and Peak Area Error	The coefficient of variation (CV) cannot be calculated for the affected gas, and calibration curve generation is terminated.	Review the Peak Areas Table for missing, zero, or non-numeric values. Confirm that replicate standards are complete and properly grouped, then correct the file and re-run the analysis.

4	Column Header Error	Required columns cannot be recognized, preventing CV calculation and halting regression and curve-fitting procedures.	Rename all column headers to match the required format exactly, ensuring correct spelling, capitalization, and spacing. Save the corrected file in .xlsx format and re-upload.
4	Output Folder Duplication	Output generation is halted to prevent overwriting existing results.	Enter a unique output folder name that does not already exist in the working directory and re-submit the analysis.
4	SITE ID Mismatch	Sample alignment fails, blocking gas concentration calculations and batch processing.	Verify that SITE IDs match exactly between the SITE ID Order and Batch worksheets. Ensure SAMPLE ID values are correctly concatenated and consistent across all sheets, then re-upload the corrected Preparation File.
4	No Valid Combination to Compute CV	Regression analysis cannot proceed because no valid standard combinations are detected, and calibration curves are not generated.	Confirm that standard identifiers are present and consistent in both the Preparation File and Peak Areas Table. Ensure replicate standards are correctly grouped and meet internal validation criteria, then re-run the module.
5	Column name differences and/ sheet name differences	The DASIG-FLUX module cannot validate the input file and halts processing due to inconsistent column	Ensure that all column headers and worksheet names in the concentrations table file exactly match the required template, including correct spelling, symbols, and formatting.

		headers or worksheet names.	
5	Duplicate Output Folder Name	The module does not execute to prevent overwriting existing results.	Provide a unique output folder name that does not already exist in the selected working directory.
5	Data error in PPM INPUT sheet	Anomalous data entries prevent the module from generating output.	Verify and correct SITE IDs in the PPM INPUT sheet based on the experimental design. Modify any SITE IDs flagged by the DASIG-FLUX module before re-running the analysis.
5	Missing SITE IDs detected in the HEADSPACE INPUT sheet	The model cannot run properly due to incomplete sample identification.	Provide correct and consistent SITE IDs that match across both the HEADSPACE INPUT and PPM INPUT sheets.
5	Missing data input	If processing continues with missing values, no output files are generated.	Identify and correct missing values in the input file before re-running the module.
5	Incorrect TRT IDs in HEADSPACE INPUT sheet	Inconsistent TRT IDs may propagate errors into downstream GWP calculations, resulting in inaccurate outputs.	Verify that TRT IDs and associated metadata are consistent throughout all input files used in the FLUX analysis.
5	Data error: Invalid flux output values	Zero CO_2-C flux values are flagged as physically unrealistic under field	Users may proceed while retaining zero CO_2-C values for exploratory purposes or cancel processing to correct source files and rerun the module. Review SITE IDs associated with zero

		conditions and may compromise cumulative flux and GWP calculations.	CO_2-C outputs, check concentration linearity over the sampling period, verify field conditions, sample integrity, and vial handling, and reanalyze samples if necessary.
6	Fewer than two FLUX result files selected	The DASIG-GWP module cannot organize results by treatment and replicate or generate treatment-level summary tables, and processing is halted.	Add at least one additional DASIG-FLUX result file and rerun the module, as a minimum of two files is required for treatment grouping and summary output generation.
6	Zero CO_2-C flux values detected	CO_2-C flux values equal to zero are physically unrealistic under field conditions using vented chambers and may bias cumulative emissions and GWP calculations.	Review the flagged records and verify source data. Users may correct the input files and rerun the model or proceed with the flagged values if they are confirmed to be valid.
6	Empty or unreadable FLUX result file	The GWP module cannot process files with no valid data records, and execution is stopped to prevent incomplete or invalid output.	Replace the empty or unreadable file with a valid DASIG-FLUX result workbook and rerun the GWP module.
6	Non-numeric values in flux columns	Text entries, blanks, or invalid characters in the CH_4-C, N_2O-N, or CO_2-C	Correct all non-numeric entries in the affected FLUX result files, reload the corrected files into the DASIG-GWP module, and rerun the analysis.

		columns prevent numerical integration and GWP calculations.	