

MUCalc 4.0 — Measurement Uncertainty Calculator User Manual

1. Introduction

Welcome to MUCalc 4.0, a comprehensive web-based measurement uncertainty calculator specifically designed for chemical analysis. This user guide will help you navigate through the software's features and functionalities, providing step-by-step instructions for calculating measurement uncertainty using internationally recognized statistical methods.

MUCalc 4.0 is developed by the Leverhulme Research Centre for Forensic Science (LRCFS) and funded by The Leverhulme Trust (RC-2015-011).

2. What is Measurement Uncertainty?

Measurement uncertainty is a parameter that characterizes the dispersion of values that could reasonably be attributed to a measurement. In chemical analysis, uncertainty estimation is essential for:

- Quality assurance in analytical laboratories
- Accreditation compliance (ISO/IEC 17025)
- Risk assessment in forensic science
- Validation of analytical methods
- Confidence interval determination for reported results

MUCalc 4.0 provides a systematic approach to quantifying measurement uncertainty by evaluating multiple uncertainty components and combining them according to the Guide to the Expression of Uncertainty in Measurement (GUM).

There are two methods commonly used for the measurement of uncertainty estimation: the top-down and the bottom-up method. MUCalc 4.0 implements the bottom-up approach.

3. Key Features of MUCalc 4.0

- **Comprehensive Uncertainty Evaluation:** Calculate uncertainty components from homogeneity, method precision, calibration curve, calibration standard, and sample preparation.
- **Statistical Methods:** Support for linear and quadratic calibration curves with weighted least squares regression for linear calibration.
- **Detailed Workings Display:** View step-by-step calculations for each uncertainty component.
- **Visualizations:** Charts and graphs for uncertainty budget analysis.
- **Save and Load Functionality:** Save complete calculation sessions for future reference.
- **Homogeneity Testing:** Standalone homogeneity analysis using ANOVA.

- **Export Capabilities:** Download calculation reports and results.

4. System Requirements

- **Web Browser:** Google Chrome (recommended), Firefox, Edge, or Safari (latest versions)
- **Internet Connection:** Required for initial access
- **Screen Resolution:** At least 1280×720 for optimal experience
- **JavaScript:** Must be enabled
 - **Google Chrome:** Settings → Privacy and Security → Site Settings → JavaScript → "Sites can use JavaScript"
 - **Firefox:** Type `about:config` in the address bar, search for `javascript.enabled`, and set it to `true`
 - **Microsoft Edge:** Settings → Cookies and site permissions → JavaScript → Toggle on

5. Accessing the Software

1. Open your web browser
2. Navigate to the MUCalc 4.0 URL provided by your administrator
3. You will be directed to the home page

6. Home Page Overview

After accessing MUCalc 4.0, you will see the welcome screen. Its features are described below.

Navigation Bar (top of screen):

- MUCalc 4.0 logo and branding
- LRCFS and Leverhulme Trust logos

Welcome Section

- Main title "Welcome to MUCalc 4.0"
- Brief description of the calculator's purpose
- "Get Started" button for quick access
- "Help" button for assistance

Features Overview — displays the main components:

- **Homogeneity** — Calculate uncertainty due to inhomogeneity in the sample
- **Method Precision** — Calculate uncertainty from analytical method variability
- **Calibration Curve** — Determine uncertainty from linear and quadratic calibration
- **Homogeneity Testing** — Statistical analysis of sample homogeneity
- **Combined Uncertainty** — Compute combined and expanded uncertainty

Footer

- Development credits (LRCFS)

- Funding information (Leverhulme Trust)
- Copyright information

7. Measurement Uncertainty Calculation Workflow

MUCalc 4.0 follows a four-step workflow for calculating measurement uncertainty:

Step	Description
Step 1	Input Case Sample Data
Step 2	Upload Data
Step 3	Calculate
Step 4	Results

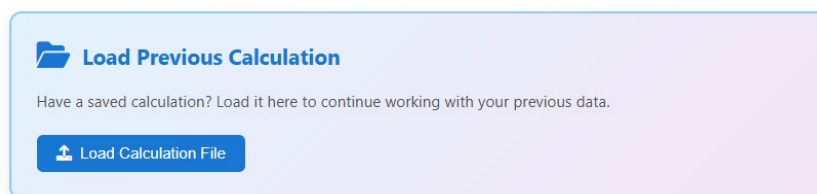
8. Case Sample Data Page

Click the "Get Started" button on the home page to begin. You will be taken to the Measurement Input Parameters page.

Load Previous Calculation

If you have a previously saved calculation file (.mucalc format):

4. Click the "Load Calculation File" button in the "Load Previous Calculation" section
5. Browse and select your .mucalc file
6. The system will:
 - Restore all measurement parameters
 - Populate uploaded data files
 - Display upload status
 - Allow you to proceed directly to calculation or modify data



Case Sample Data

Mean Concentration (x_s):

- Description: The mean concentration value of your case sample
- Input: Numerical value (decimal allowed)

- Units: Select from dropdown menu:

- mg/L (milligrams per liter)
- $\mu\text{g/L}$ (micrograms per liter)
- ng/L (nanograms per liter)
- ppm (parts per million)
- ppb (parts per billion)
- % (percentage)
- mol/L (moles per liter)
- Custom (specify your own unit)

- Example: 2.5 mg/L

Number of Replicates (r_s):

- Description: Number of replicate measurements performed on the case sample
- Input: Whole number between 1 and 100
- Typical range: 1–10
- Example: 3

 **Case Sample Data**

Mean Concentration (x_s) 

mg/L

▼

This is the measured concentration of your case sample, used as the baseline for uncertainty calculations.

Number of Replicates (r_s) 

3

Coverage Factor Method

You can choose between two methods:

Option A: Specify Confidence Level (Default)

- Select a confidence level (CL%) for the uncertainty calculation
- Preset options: 90%, 95% (default), 99%
- Custom: Enter any value between 50% and 99.99%
- The system will automatically calculate the coverage factor using the t-distribution

Option B: Specify Coverage Factor Directly

- Directly enter the coverage factor (k) value
- Input range: 1 to 10
- Step: 0.01
- Common values:

- $k = 1.96$ (approximately 95% confidence level for normal distribution)
- $k = 2.58$ (approximately 99% confidence level for normal distribution)
- $k = 2.00$ (common choice for practical uncertainty reporting)

Navigation

- **Back:** Return to the home page
- **Reset Form:** Clear all entered data
- **Continue to Data Upload:** Proceed to Step 2 (validates that all required fields are completed)

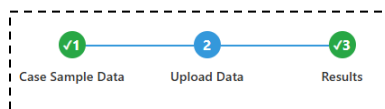
8. Upload Uncertainty Data Page

After entering the measurement parameters, you proceed to the Data Upload page.

Overview

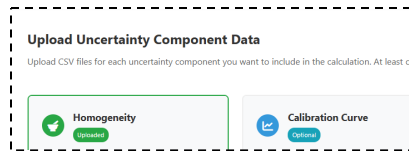
The Data Upload page displays:

- **Progress Indicator:** Shows you are on Step 2 of 3

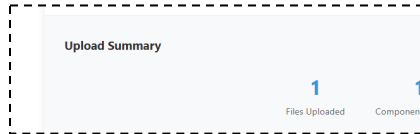


- **Case Sample Data Summary:** Reviews the parameters entered in Step 1

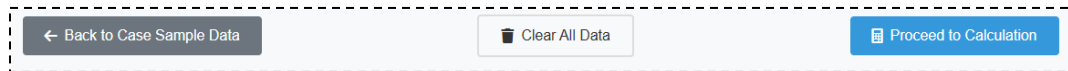
- **Upload Uncertainty Component Data:** Main section for uploading CSV files



- **Upload Summary:** Statistics on files uploaded



- **Navigation Buttons:** Back to Case Sample Data, Clear All Data, Proceed to Calculation



⚠ Important — Data Format Requirement

MUCalc will only produce accurate results when the uploaded CSV files follow the **exact column headers and data structure** shown in the downloadable example files for each component. Data files with different column names, additional columns, or a different layout may produce inaccurate or unexpected results. Please download and review the example CSV for each component before uploading your data.

Uploading Uncertainty Components

MUCalc 4.0 supports five uncertainty components. At least one component must be uploaded to proceed with calculations. Each component is optional, allowing you to include only the relevant sources of uncertainty for your analysis.

Component 1: Homogeneity

Purpose: Calculate uncertainty due to inhomogeneity in the sample and perform homogeneity testing.

File Requirements:

- Format: CSV (Comma-Separated Values)
- Expected columns: **Group**, **Replicate**, **Concentration**
- Example structure:

```
Group,Replicate,Concentration
1,1,2.45
1,2,2.48
2,1,2.52
2,2,2.50
```

Note: The group values can also be a single word, e.g. Sample_A, Sample_B.

How to Upload

- Click on the Homogeneity upload area or drag and drop a CSV file
- The system validates the file format
- File details (name, size, number of rows) are displayed
- To remove: Click the "Remove" button

Download Example: Click "Download Example CSV" to get a template file

Component 2: Calibration Curve

Purpose: Calculate uncertainty from the calibration process used to convert instrument response to concentration.

MUCalc 4.0 supports two types of calibration curves.

Component 2.1: Linear Calibration Curve

File Requirements:

a) Calibration Curve CSV (Required)

- Expected columns: conc (x), run1 (y)
- Each row represents a calibration point
- Example structure:

```
conc,run1
0.5,0.52
1.0,1.05
2.0,2.01
4.0,3.98
5.0,5.10
```

b) Pooled Standard Error CSV (Optional)

- Used for more accurate uncertainty estimation when replicate measurements exist at each calibration level
- Expected columns: Concentration, Standard_Error
- Example structure:

Concentration,Standard_Error
1.0,1.02
1.0,1.05
1.0,1.08

Weight Selection

Choose the weighting scheme for weighted least squares (WLS) regression:

Weight	Description
Default (1)	Unweighted regression (ordinary least squares)
Concentration (1/x)	Weight inversely proportional to concentration
Concentration Squared (1/x ²)	Weight inversely proportional to concentration squared (recommended for heteroscedastic data)
Peak Area (1/y)	Weight inversely proportional to peak area ratio (requires Mean Peak Ratio)
Peak Area Squared (1/y ²)	Weight inversely proportional to peak area squared (requires Mean Peak Ratio)
Custom Weights	Enter a custom weight value (W _s)

Custom Weight Value (W_s): Required when "Specify custom Weights" is selected. Input: Numerical value.

Component 2.2: Quadratic Calibration Curve

File Requirements

Calibration Curve CSV (Required)

- Expected columns: Conc (x), run1 (y)
- Similar to linear calibration but fitted with a quadratic model ($y = a + bx + cx^2$)

Mean Peak Ratio (y_s) (If required)

- The mean peak area ratio for your case sample
- Used in the uncertainty calculation
- Input: Numerical value

Note: Quadratic calibration does not currently support pooled standard error data.

Switching Between Linear and Quadratic:

- Use the tab buttons at the top of the Calibration Curve section
- Click "Linear Fit" or "Quadratic Fit" to switch
- Each tab has its own file upload areas

Remove Calibration Data:

- Click "Remove Calibration Curve Data" button to clear all calibration files

Component 3: Method Precision

Purpose: Calculate uncertainty due to the variability of the analytical method.

File Requirements:

- Format: CSV
- Expected columns: conc, run1, run2, run3, run4, run5, run6, run7, run8, run9, run10, run11
- Multiple concentrations with replicate runs at each level
- Example structure:

```
conc, run1, run2, run3, run4, run5, run6, run7, run8, run9, run10, run11
2, 2.198, 1.825, 2.144, 2.108, 2.065, 1.81, 1.993, 1.829, 1.786, 2.044, 1.851
2, 1.988, 1.92, 2.166, 2.052, 2.002, 1.806, 1.942, 1.768, 1.88, 1.81, 1.822
2, 2.161, 1.851, 2.182, 1.972, 2.152, 1.795, 1.931, 1.826, 1.785, 1.896, 1.701
```

How to Upload:

- Click on the Method Precision upload area or drag and drop
- System validates the file
- File details are displayed
- To remove: Click the "Remove" button

Download Example: Click "Download Example CSV"

Component 4: Calibration Standard

Purpose: Calculate uncertainty from the preparation of calibration standards.

File Requirements: Two CSV files are required.

a) Structure Data (Required)

- Contains the dilution structure and uncertainty information
- Example columns: solution, madeFrom, compoundPurity, compoundTolerance, compoundCoverage
- Example structure:

```

solution, madeFrom, compoundPurity, compoundTolerance, compoundCoverage
Ref. Std. Solution      1000000, 33000, 2
Stock SolutionA, Ref.Std.Solution
Working SolutionB, StockSolutionA
Working SolutionC, StockSolutionA
CalibratorsRange1, WorkingSolutionC
CalibratorsRange2, WorkingSolutionB

```

b) Equipment Data (Required)

- Contains equipment specifications and calibration uncertainties
- Example columns: Solution, equipment, equipmentVolume, equipmentTolerance, equipmentCoverage, equipmentTimesUsed
- Example structure:

```

solution, equipment, equipmentVolume, equipmentTolerance, equipmentCoverage,
equipmentTimesUsed
Stock Solution A, pipette, 25, 0.3, 2, 1
Stock Solution A, pipette, 1000, 5, 2, 2

```

How to Upload:

- Upload Structure CSV in the first upload area
- Upload Equipment CSV in the second upload area
- Both files must be uploaded for this component
- To remove: Click individual "Remove" buttons or "Remove All"

Download Examples: Click "Structure Example" or "Equipment Example"

Component 5: Sample Preparation

Purpose: Calculate uncertainty from sample preparation procedures (weighing, dilutions, volumetric operations).

File Requirements:

- Format: CSV
- Contains equipment information and uncertainties
- Example columns: Equipment, EquipmentCapacity, EquipmentCapacityTolerance, EquipmentCoverage, EquipmentTimesUsed
- Example structure:

```
equipment,equipmentCapacity, equipmentCapacityTolerance, equipmentCoverage,  
equipmentTimesUsed  
Pipette, 1000, 5, 2, 1  
Volumetric Flask, 100, 0.1, 2, 1  
Balance, 205, 0.00015, 2, 1
```

How to Upload

- Click on the Sample Preparation upload area or drag and drop
- System validates the file
- File details are displayed
- To remove: Click the "Remove" button

Download Example: Click "Download Example CSV"

Upload Summary

The Upload Summary section displays real-time statistics:

- **Files Uploaded:** Total number of CSV files uploaded
- **Components Selected:** Number of uncertainty components included
- **Total Data Points:** Cumulative data points across all files

Requirements Note: At least one uncertainty component must be uploaded to proceed.

Navigation and Actions

- **Back to Case Sample Data:** Return to Step 1 to modify input parameters
- **Clear All Data:** Remove all uploaded files (confirmation required)
- **Proceed to Calculation:** Validates uploads and advances to Step 3
 - Button is disabled until at least one component is uploaded
 - Clicking sends data to the server and initiates calculations

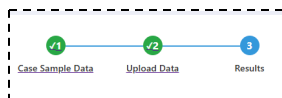
9. Uncertainty Calculation Page

After uploading your data, clicking "Proceed to Calculation" takes you to the Calculation page.

Automatic Processing

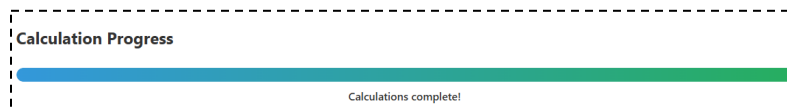
The calculation page shows the following components.

Progress Indicator: Step 3 is active.



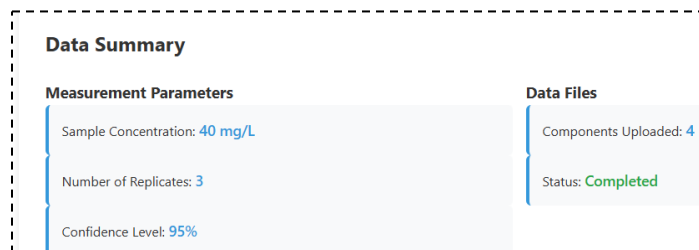
Calculation Progress Bar

- Visual progress bar (0–100%)



- Status messages updating in real-time
 - "Initializing calculations..."
 - "Processing uploaded files..."
 - "Running uncertainty calculations..."
 - "Calculating combined uncertainty..."
 - "Computing expanded uncertainty..."
 - "Generating results..."
 - "Calculations complete!"

Data Summary: Reviews the uploaded files and parameters



The backend performs the following calculations.

- Validates all uploaded data
- Runs individual component calculations
- Computes combined uncertainty
- Determines coverage factor
- Calculates expanded uncertainty
- Generates visualisations

Processing Time: Typically 2–10 seconds depending on data size.

Results

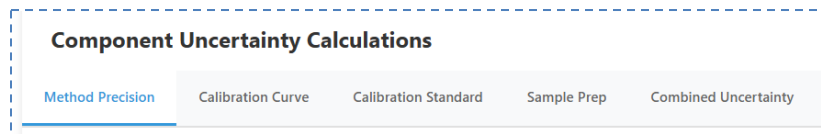
Upon successful completion, the results are displayed automatically organized in separated pages accessed with tabs. The tabs below are for a calculation where only homogeneity data has been uploaded.

Component Uncertainty Calculations

Each uncertainty component that was uploaded is displayed in a tabbed interface.

Tab Navigation:

- Click on each tab to view results for that component
- Active tab is highlighted



- Each tab header shows a "Show Workings" button:



Show Workings Feature

For transparency and educational purposes, MUCalc 4.0 provides detailed step-by-step calculations for each component.

How to Use

7. Click the "Show Workings" button next to any component tab
8. A modal window (see picture below) opens displaying
 - Component name in the header
 - Detailed calculation steps
 - Formulas with mathematical notation
 - Intermediate values
 - Tables with data breakdowns
 - Final results highlighted

Detailed Workings: Method Precision

Method Precision Uncertainty - Detailed Calculations

Method

The relative standard uncertainty method for a nominal concentration NV. The relative standard uncertainty assigned to x_s is the relative standard uncertainty of the NV which is the closest to x_s .

The Relative Standard Uncertainty of method precision is given by:

$$u_r(\text{MethodPrec})_{(NV)} = \frac{u(\text{MethodPrec})_{(NV)}}{\bar{x}_{(NV)}}$$

where

$$u(\text{MethodPrec})_{(NV)} = \frac{S_{p(NV)}}{\sqrt{r_s}}$$

and pooled standard deviation

Close
Print

9. Scroll through the workings
10. Click "Print" to print the workings
11. Click "Close" or click outside the modal to close

Available for

- Homogeneity
- Method Precision
- Calibration Curve (Linear and Quadratic)
- Calibration Standard
- Sample Preparation
- Combined Uncertainty

Results Display by Component

Homogeneity Results

Displayed Information

- Standard Uncertainty (u): Absolute uncertainty value
- Relative Standard Uncertainty (u_r): As a decimal

Show Workings Content

- Parameters (N, k, α , observations per group)
- Grand Mean calculation
- Mean Sum of Squares Between (MSSB) with group details
- Sum of Squares Within (SSW) with individual calculations
- Mean Sum of Squares Within (MSSW)
- Standard Uncertainty formula and calculation
- Relative Uncertainty (highlighted result)

Method Precision Results

Displayed Information

- Pooled Standard Deviation (S_p): Pooled standard deviation across concentrations
- Mean Concentration ($\bar{x}$): Mean of all concentration levels
- Standard Uncertainty (u): Calculated as $S_p / \sqrt{r_s}$
- Relative Standard Uncertainty (u_r): $u / \bar{x}$
- Relative Standard Uncertainty (%): $u_r \times 100\%$
- Degrees of Freedom (v): Total degrees of freedom
- Concentrations Tested: List of concentration levels

Show Workings Content

- Parameters summary (concentrations, runs, target concentration, r_s)
- Step-by-step calculation table (Nominal Value, Run, Mean, Std Dev, DOF, $S^2 \times v$)
- Sum of Degrees of Freedom ($\sum v$)
- Sum of $S^2 \times v$
- Pooled Standard Deviation (S_p) calculation with formula
- Standard Uncertainty (u) calculation
- Relative Uncertainty (u_r) with final result highlighted

Calibration Curve Results

For Linear Calibration:

Displayed Information:

- Regression Equation: $y = a + bx$ (with coefficients)
- Slope (b_1): Regression slope
- Intercept (b_0): Regression intercept
- R^2 : Coefficient of determination
- Standard Error (S_{yx}): Residual standard error

- Weighted Mean X ($\bar{x}_w$): For weighted regression
- Standardised Weight (W_s): Weight of case sample
- Standard Uncertainty (u): Absolute uncertainty
- Relative Standard Uncertainty (u_r): Decimal and percentage
- Degrees of Freedom (v): Regression degrees of freedom
- Weight Type: Applied weighting scheme

For Quadratic Calibration:

Displayed Information

- Regression Equation: $y = a + bx + cx^2$ (with coefficients)
- Quadratic Coefficient (c): Second-order term
- Linear Coefficient (b): First-order term
- Intercept (a): Constant term
- R^2 : Coefficient of determination
- Standard Error (Sy): Residual standard error
- Standard Uncertainty (u): Absolute uncertainty
- Relative Standard Uncertainty (u_r): Decimal and percentage
- Degrees of Freedom (v): Regression degrees of freedom

Show Workings Content

- Parameters (curve type, weighting, number of points, DOF)
- Regression equation with coefficients
- Calibration data table
- Weighted calculations (if applicable)
- Pooled standard error (if provided)
- Uncertainty formula breakdown
- Standard uncertainty calculation
- Relative uncertainty (highlighted)

Calibration Standard Results

Displayed Information

- Structure Table: Dilution steps with values and uncertainties
- Equipment Table: Equipment specifications and tolerances
- Uncertainty Budget: Contribution from each source

Show Workings Content

- Preparation structure breakdown
- Equipment uncertainty contributions
- Distribution types (Normal, Rectangular, Triangular)
- Divisors applied for each distribution
- Combined uncertainty calculation
- Relative uncertainty

Sample Preparation Results

Displayed Information

- Equipment Table: List of equipment with uncertainties
- Operations: Weighing, dilution, volume transfer operations
- Total Equipment Count
- Individual Uncertainties

Show Workings Content

- Equipment list with specifications
- Uncertainty values and distributions
- Divisor calculations
- Combined uncertainty formula
- Step-by-step combination
- Final relative uncertainty

Combined Uncertainty

After individual component results, the Combined Uncertainty section displays the aggregated uncertainty from all active components.

Combined Standard Uncertainty:	3.167624
Coverage Factor:	1.960
Confidence Level:	95.0%

Show Workings Button: Available for combined uncertainty to show:

- List of active components
- Individual relative uncertainties

- Sum of squares calculation
- Combined relative uncertainty
- Combined absolute uncertainty ($uc = x_s \times uc,r$)

Uncertainty Breakdown Table

Component Breakdown				
Component	Uncertainty Value	Relative (%)	Squared Contribution	Contribution to Combined
Method Precision	0.013672	1.3672%	0.00018692	10.5%
Calibration Curve	0.026329	2.6329%	0.00069323	20.2%
Calibration Standard	0.070666	7.0666%	0.00499375	54.1%
Sample Preparation	0.019931	1.9931%	0.00039725	15.3%
Total (Combined)	0.079191	7.9191%	0.00627115	100.0%

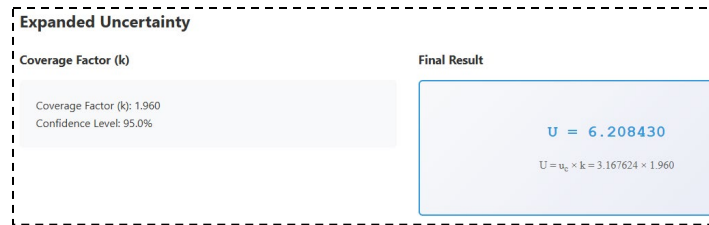
Coverage Factor

The coverage factor section provides the coverage factor that is used. If the coverage factor is calculated, the component used for its calculation are displayed.

Coverage Factor Calculation	
Effective Degrees of Freedom:	2436.6
Coverage Factor (k):	1.960
Component Degrees of Freedom	
Method Precision: 10.0	Calibration Curve: 38.0
Calibration Standard: Infinity	Sample Preparation: Infinity

Expanded Uncertainty and final result

The Expanded Uncertainty section provides the final uncertainty calculation with the coverage factor applied.



Uncertainty Budget Chart

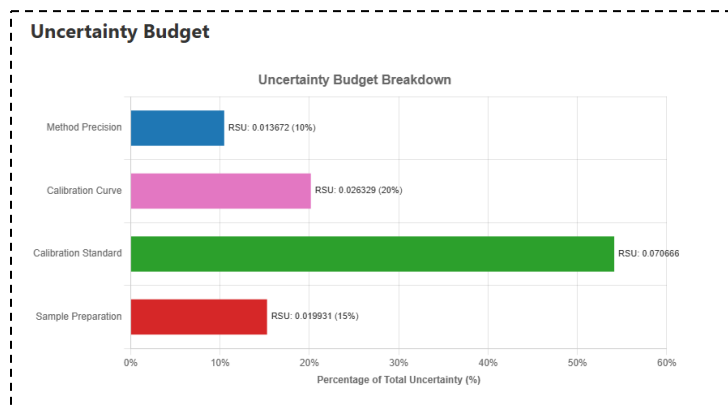
A visual representation of the uncertainty budget is displayed as a bar chart.

Bar Chart:

- Each bar represents a component's percentage contribution
- Colors distinguish each component
- Hover over bars to see exact values

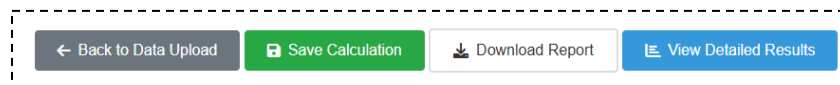
Chart Legend:

- Lists all components with colors
- Shows contribution percentages



Action Buttons

At the bottom of the results page, several action buttons are available.



Back to Data Upload

- Returns to Step 2
- Allows you to modify uploaded files or add/remove components
- Previous calculation results are cleared

Save Calculation

- Opens a modal dialog
- Enter a name for your calculation
- Saves all parameters, uploaded data, and results to a .mucalc file
- Downloads the file to your computer
- File format: JSON containing complete calculation state
- Can be loaded later from the Data Upload page

Download Report

- Generates a comprehensive PDF or Excel report
- Includes all parameters, data, results, and charts
- Suitable for documentation and archiving

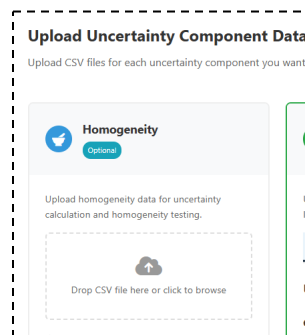
View Detailed Results

- Expands all component results
- Shows additional statistical details
- Provides export options for individual components

10. Standalone Homogeneity Testing

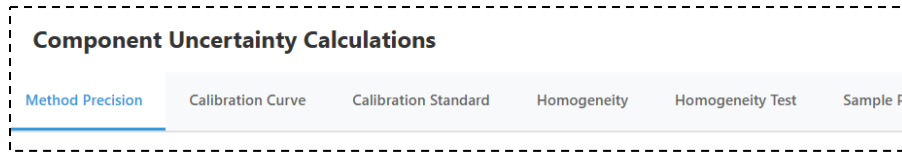
MUCalc 4.0 includes a dedicated Homogeneity Testing module accessible from the main navigation menu. The test uses the same data as for the homogeneity uncertainty component.

Upload data in the “Upload Uncertainty Data” page



Homogeneity Test Calculation

The calculations for the homogeneity tests are performed when the homogeneity data is uploaded. The results can be found in the tab for “Homogeneity Test”.



13.4 Contact and Support

- **Developed by:** Leverhulme Research Centre for Forensic Science (LRCFS)
- **Funded by:** The Leverhulme Trust (RC-2015-011).
- **Version:** 4.0
- **Copyright:** © 2025 LRCFS. All rights reserved.

For technical support, please contact your system administrator or the LRCFS development team.