

# User Guide for Software Engineering: Alkalytics

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# 1 Introduction

This comprehensive document provides complete instructions for installing, configuring, and using all features of the Alkalytics web application.

## 2 System Overview

This section describes the technical architecture, components, and requirements for running Alkalytics.

### 2.1 Detailed Requirements

Lists all hardware and software requirements for running the application.

Component	Minimum	Recommended
RAM	8GB	16GB
Storage	5GB	50GB SSD
Processor	2 cores	4 cores

#### Hardware Requirements

## 3 Installation Guide

This section provides complete step-by-step instructions for setting up the Alkalytics environment.

### 3.1 Step-by-Step Installation

#### 1. Prerequisite Installation

- (a) Install Node.js from <https://nodejs.org>
- (b) Install MongoDB from <https://www.mongodb.com>
- (c) Install Python 3.x from <https://www.python.org>

#### 2. Repository Setup

```
git clone https://github.com/SumanyaG/Alkalytics.git
```

### 3. Dependency Installation

```
yarn install  
pip install -r requirements.txt
```

### 4. Database Configuration

- (a) KATE HELP

### 5. Application Launch

- (a) Start backend:

```
uvicorn api:app --reload --host 127.0.0.1 --port 8000
```

- (b) Start server:

```
yarn ts-node src/utils/server.ts
```

- (c) Start frontend:

```
yarn start
```

## 3.2 Verification

After installation, verify all components are running:

1. Frontend: `http://localhost:3000`
2. Server: `http://localhost:8000/graphql`
3. Backend: `http://localhost:8000/docs`
4. Database: Check MongoDB connection on port 27017

## 4 User Management

### Section Overview

This application has different user roles. Each role has a different set of permissions and respective capabilities within the application.

#### 4.1 Admin and Researcher Role

Administrators have full control over all system functionality including data management, user configuration, and system settings. Both Admin and Researcher roles have the same permissions.

These features include:

- Editing tables, including modifying cells, adding/removing rows and columns.
- Setting data types for columns.
- Using the Excel function bar for calculations.
- Computing efficiency metrics.
- Managing bulk data uploads.
- Generating and exporting graphs.

#### 4.2 Researcher Assistant Role

Researcher assistants can view data, run analyses, and generate reports but have limited system configuration capabilities.

These features include:

- Viewing and searching tables (Experiment, Efficiency, and Raw Data).
- Searching within a specific column or the entire table.
- Generating graphs but with restricted data modification capabilities.

## 5 Web Application Pages

### 5.1 Login and Sign Up Process

When users first load onto the page, they will be greeted by a log in screen. If the user has login credentials, log in as normal

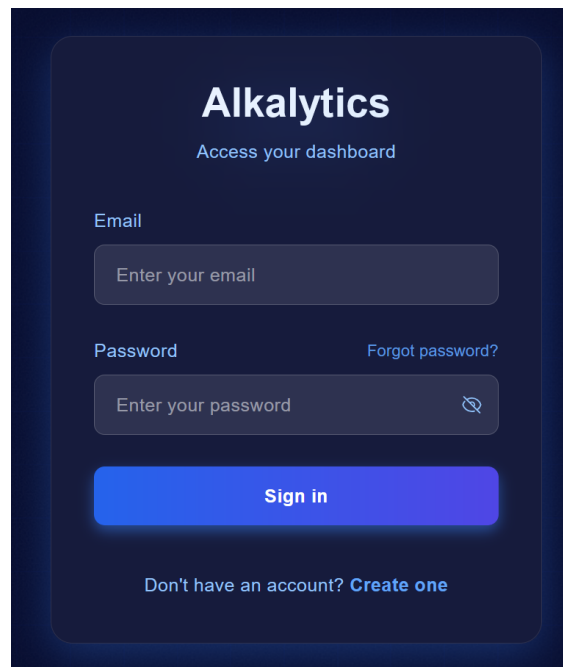
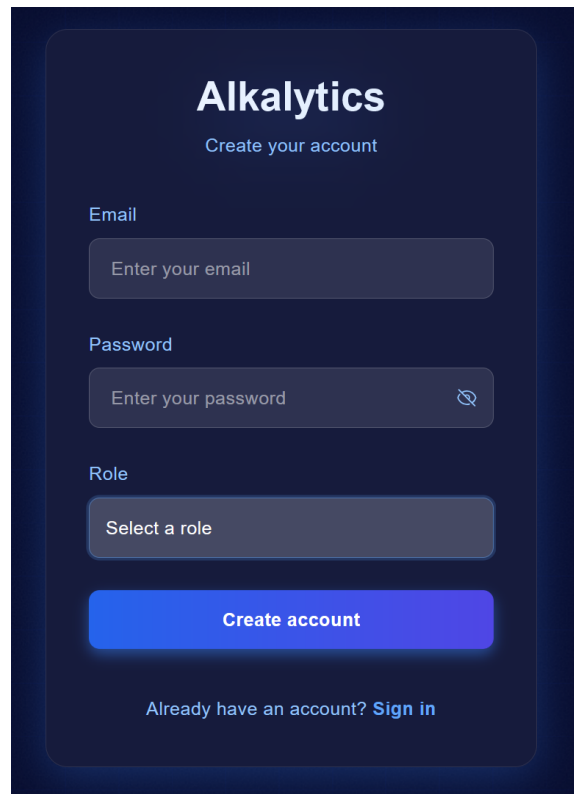
The image shows a login form for 'Alkalytics'. At the top, the word 'Alkalytics' is displayed in a large, bold, white font, with the tagline 'Access your dashboard' in a smaller, lighter blue font below it. The form consists of two input fields: 'Email' and 'Password'. The 'Email' field has a placeholder text 'Enter your email'. The 'Password' field has a placeholder text 'Enter your password' and a small eye icon to its right. Above the password field, there is a link 'Forgot password?'. Below the input fields is a large, rounded blue button with the text 'Sign in' in white. At the bottom of the form, there is a link 'Don't have an account? Create one' in a light blue font.

Figure 1: Login Form

### 5.2 Sign Up Process

If users do not have an account, they will need to create one by clicking the **Create one** button at the bottom of the login form. The user must then enter an email and desired password. There will be three roles to pick from, Admin, Researcher and Research Assistant. After creating a user account, log in as normal.

The image shows a sign-up form for 'Alkalytics' on a dark blue background. The form is centered and contains the following elements: the brand name 'Alkalytics' in white, the text 'Create your account' below it, three input fields for 'Email', 'Password', and 'Role' (each with a placeholder text), a blue 'Create account' button, and a link 'Sign in' for users who already have an account.

**Alkalytics**  
Create your account

Email  
Enter your email

Password  
Enter your password

Role  
Select a role

Create account

Already have an account? [Sign in](#)

Figure 2: Sign Up Form

## 5.3 Dashboard

The Dashboard provides a quick, interactive, and structured overview of the most recent key data insights through visualizations and tables. It is designed to help users analyze trends, monitor performance, and interact with data efficiently.



Figure 3: Dashboard Overview

### 5.3.1 Key Features

- **Graphs:** Displays visual representations of data trends and relationships.
- **Data Tables:** Organizes numerical and analytical data in a structured format, allowing for sorting, filtering, and searching.
- **Navigation Panel:** A sidebar with quick access to different sections of the platform, including:
  - Dashboard
  - Data View
  - Upload
  - Graphs
  - Logout

## 5.4 Upload

The upload functionality allows users to efficiently import files in various formats for analysis. This section outlines the steps for uploading files, the types of files supported, and best practices to ensure a smooth upload experience.



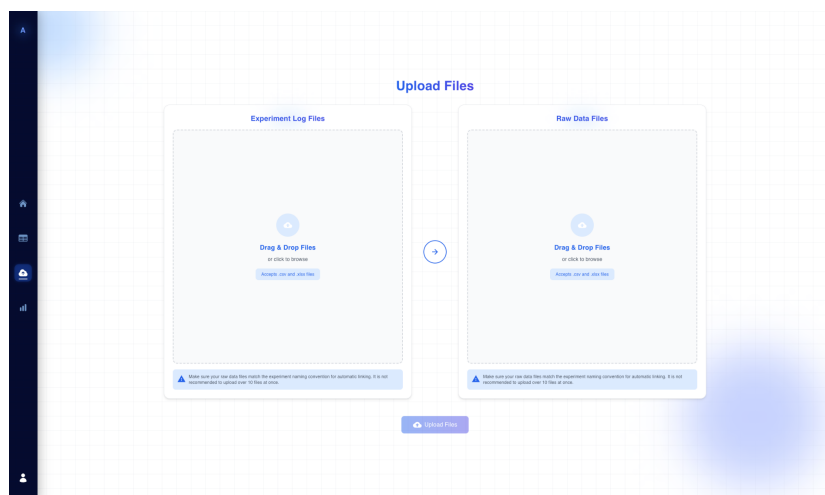


Figure 4: Upload Files Interface

#### 5.4.1 Step-by-Step Upload

To upload files, follow these steps:

1. Navigate to the Upload Page.
2. Select the file type you wish to upload: either **Experiment Log** or **Raw Data**.
3. Choose your preferred upload method:
  - **Drag and Drop:** Drag files directly into the designated upload area.
  - **Browse and Select:** Click on the upload box to open a file browser and select files manually.
4. Click the **Upload** button to initiate the upload process.

#### 5.4.2 Linking Raw Data Files to Experiments

In some cases, the migration algorithm may not be able to automatically link a raw data file to its corresponding experiment. When this occurs, users will be prompted to manually match the data file with the appropriate experiment ID.

**Link Data Files**

**Ambiguous Data Requires Matching**  
Please match each data file with the corresponding experiment id.

**Data Id**

20240531.xlsx

**Possible Matching Experiment Id**

#66 2024-05-31    #67 2024-05-31

1 of 1

**Submit**

Figure 5: Link Data Files Prompt

When presented with this prompt, users should:

1. Review the displayed Data ID to ensure it corresponds to the correct file.
2. Select the appropriate Experiment ID from the provided options.
3. Click the **Submit** button to confirm the link.

This manual linking process ensures that all data files are accurately associated with their respective experiments, maintaining data integrity and facilitating effective analysis.

#### 5.4.3 File Requirements

To ensure successful uploads, please adhere to the following file requirements:

Requirement	Specification
File Size	Maximum 10MB per file
Date Format	YYYY-MM-DD
Special Characters	Avoid at all costs

#### 5.4.4 File Upload Types

The upload interface categorizes files into two primary types to facilitate structured data management:

- **Experiment Log Files:** Processed logs containing IDs, dates, and input parameters.
- **Raw Data Files:** Experimental data outputted by the machine, including IDs, dates, and results.

#### 5.4.5 Supported File Formats

The following file formats are supported for upload:

- **CSV (.csv):** A structured data format using comma-separated values.
- **Excel (.xlsx):** A spreadsheet format that supports multiple sheets and structured data.

#### 5.4.6 Upload Guidelines

To maintain system performance and ensure proper data processing, users should follow these best practices:

- Limit uploads to a maximum of 10 files at once.
- Ensure that data structures match the expected formats to prevent processing errors.
- If a file does not meet the required format, the system may issue a warning or reject the upload.

## 5.5 Data View

The Data View section provides users with a structured and interactive way to explore the data uploaded into the system.

### 5.5.1 Common Functionalities

Across all tables, users can utilize the following common functionalities to enhance their data exploration experience:

- **Search:** Locate specific data points quickly using the dynamic search bar. Users can search across the entire dataset or within a single column by selecting the desired field from the dropdown menu.
- **Sorting:** Organize data systematically by clicking on any column header to sort entries in ascending or descending order. Sorting indicators (arrows) will reflect the current order.
- **Highlighting Matches:** Relevant data points are automatically highlighted upon search, drawing immediate attention to key results.
- **Row Filtering:** Non-matching rows are temporarily removed from view, simplifying the focus on pertinent data.
- **Column Navigation:** Each column is labeled alphabetically (A, B, C, etc.) for easy reference, ensuring that users can quickly identify and focus on specific data fields.

### 5.5.2 Experiment Table

The Experiment Table provides comprehensive oversight of all experiment-related data. This table allows full control over data management, including editing and deleting entries, making it an essential tool for maintaining data accuracy and integrity.



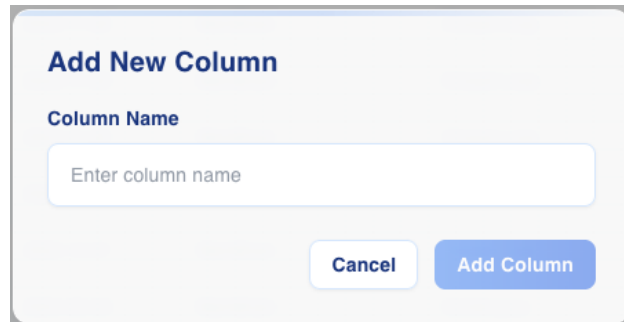
A dialog box titled "Add New Column" with a light gray background and rounded corners. Below the title is the label "Column Name" in a bold, dark blue font. Underneath the label is a white text input field with a light blue border and the placeholder text "Enter column name". At the bottom right of the dialog are two buttons: a white "Cancel" button with a light blue border and a blue "Add Column" button with white text.

Figure 7: Add New Column Dialog

**Add Row** The Add Row feature enables users to insert a new row into the table for additional data entries.

1. Click the "Add Row" button.
2. A form will appear, prompting you to enter values for each column.
3. Fill in the required fields and click "Submit" to add the new row.

### Add New Row

EXPERIMENTID

#

#

DATE

yyyy-mm-dd

MEMBRANE

CONFIGURATION

# OF STACKS

FLOW RATE (L/H)

POTENTIAL DIFF (V)

CURRENT LIMIT (A)

FEED CONCENTRATION NACL

FEED CONCENTRATION NAHCO3

FEED CONCENTRATION NAOH

FEED CONCENTRATION HCL

FEED CONCENTRATION NA2SO4

FEED CONCENTRATION NAHCO3.1

Cancel

Submit

Figure 8: Add New Row Dialog

**Remove Column** The Remove Column feature allows users to delete an existing column from the table.

1. Click the "Remove Column" button.
2. Select the column you wish to remove from the dropdown menu.
3. Confirm your action by clicking "Remove Column."
4. Note that this operation cannot be undone.

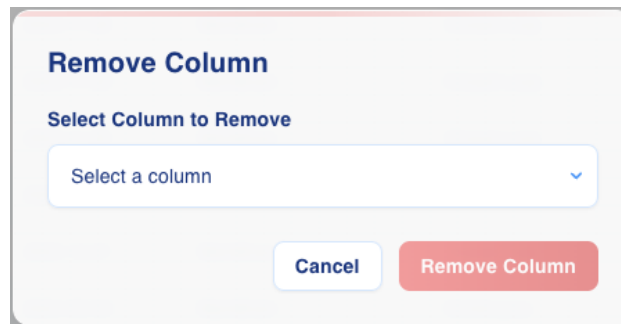


Figure 9: Remove Column Dialog

**Remove Row** The Remove Row feature enables users to delete one or more selected rows from the table.

1. Select one or more rows by checking the boxes next to them.
2. Click the "Remove Column" button.
3. Click the "Remove Row" button to open a confirmation dialog.
4. Review the warning message and click "Remove Row" again to delete the selected rows permanently.

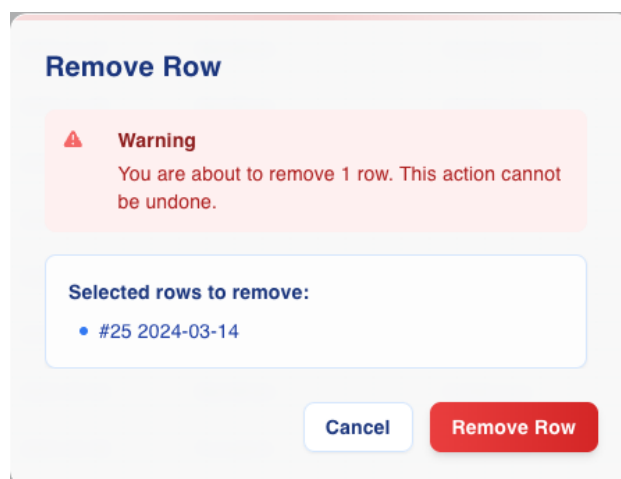
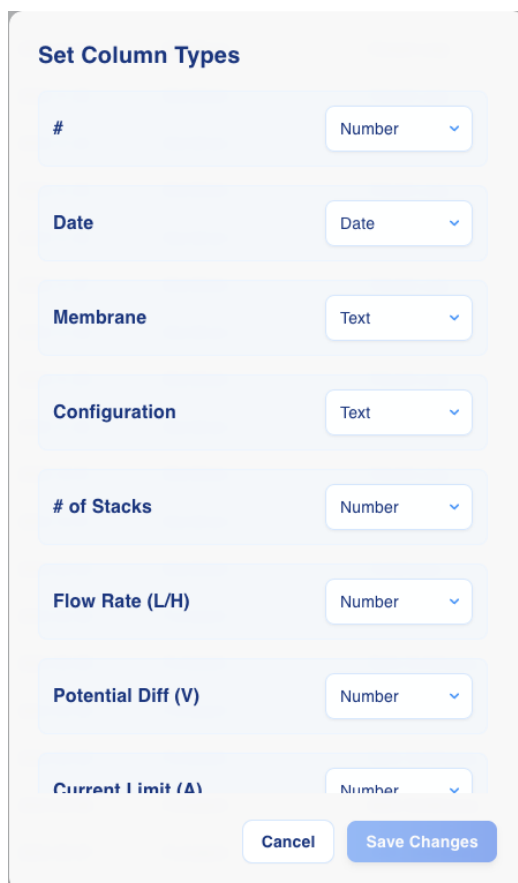


Figure 10: Remove Row Confirmation Dialog



**Set Column Types** The Set Column Types feature allows administrators to define the data type for each column in the table, ensuring consistency and accuracy.

1. Navigate to the "Set Column Types" section.
2. Select the desired data type (e.g., Number, Date, Text) for each column from the dropdown menu.
3. Click "Save Changes" to apply the updates.



The image shows a 'Set Column Types' dialog box. It has a title bar at the top. Below the title, there is a list of columns with their corresponding data types selected in dropdown menus. The columns and their types are: '#' (Number), 'Date' (Date), 'Membrane' (Text), 'Configuration' (Text), '# of Stacks' (Number), 'Flow Rate (L/H)' (Number), 'Potential Diff (V)' (Number), and 'Current Limit (A)' (Number). At the bottom right of the dialog, there are two buttons: 'Cancel' and 'Save Changes'.

Column Name	Data Type
#	Number
Date	Date
Membrane	Text
Configuration	Text
# of Stacks	Number
Flow Rate (L/H)	Number
Potential Diff (V)	Number
Current Limit (A)	Number

Figure 11: Set Column Types Dialog

**Function Bar** The Function Bar at the bottom of the table enables advanced data manipulation through calculations.

1. Select the rows you want to include in the calculation by checking the boxes next to them.
2. Choose the target column where the calculated result will be applied.
3. Enter a formula using column headers (e.g., SUM(G, I)).
4. Click the "Apply" button to calculate and update the target column with the results.

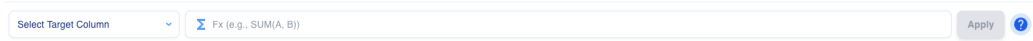
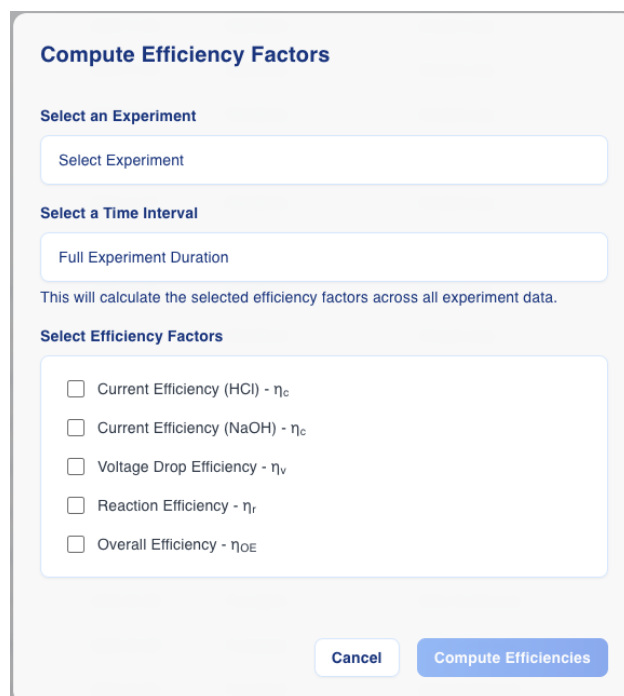


Figure 12: Function Bar

**Compute Efficiency Factors** The Compute Efficiency Factors tool enables administrators to calculate various efficiency metrics based on selected experiments and time intervals.

1. Click the "Compute  $\eta$ " button.
2. Select an experiment for which you want to compute efficiency factors.
3. Define the duration over which the calculations will be performed.
4. Select Efficiency Factor to compute.



**Compute Efficiency Factors**

**Select an Experiment**

Select Experiment

**Select a Time Interval**

Full Experiment Duration

This will calculate the selected efficiency factors across all experiment data.

**Select Efficiency Factors**

- ☐ Current Efficiency (HCl) -  $\eta_c$
- ☐ Current Efficiency (NaOH) -  $\eta_c$
- ☐ Voltage Drop Efficiency -  $\eta_v$
- ☐ Reaction Efficiency -  $\eta_r$
- ☐ Overall Efficiency -  $\eta_{OE}$

Cancel Compute Efficiencies

Figure 13: Compute Efficiency Factors Dialog

### 5.5.3 Efficiency Table (Read-Only)

The Efficiency Table offers a read-only view of efficiency metrics derived from the processed data. This table is designed to provide insights into performance trends and outcomes, enabling users to understand the effectiveness of their experiments without the ability to modify the underlying data.

### 5.5.4 Raw Data Table (Read-Only)

The Raw Data Table presents a read-only view of the raw experimental data, offering users the ability to explore detailed information captured during experiments. This table is crucial for users who need to examine individual data points and verify the integrity of the uploaded information without altering it.

## 5.6 Graph Generation

This section provides detailed instructions for creating, customizing, and exporting data visualizations.

### 5.6.1 Page Overview

The graph page is separated in two sections.

#### **Side Bar:**

On the left side of the page is the sidebar where it displays all the recently generated graphs and has the generate new graph button.

#### **Main Content:**

On the right is the main content of the page. Here, the generated graph will be displayed along with a quick linear regression analysis with a short statement of its findings

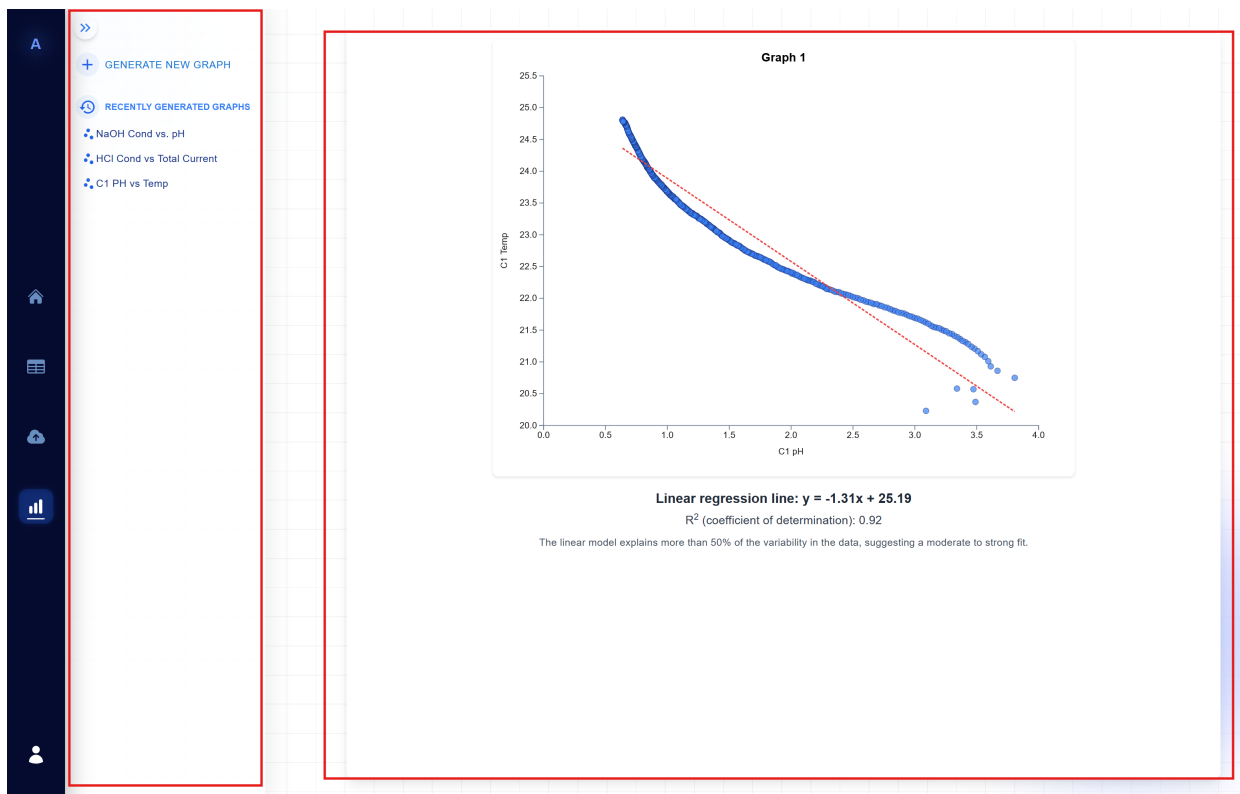


Figure 14: Graph page Separation Display

On the side bar, beside each generated graph item has an icon which signifies the type of graph it is.

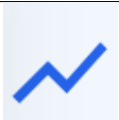


Icon	Definition
	Line Graph
	Bar Graph
	Scatter Plot

Table 1: Graph Types and Their Definitions

### Generting a New Graph:

To create a new graph, click on the **Generate New Graph** button at the top of the side bar:

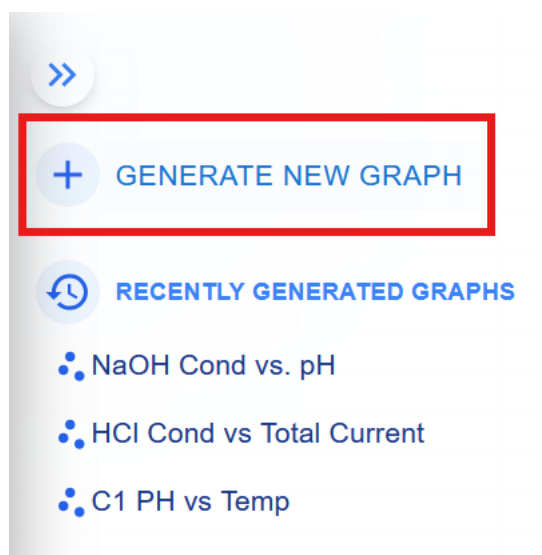


Figure 15: Highlights the Generate New Graph Button

### 5.6.2 Detailed Workflow

#### Description

There is a five-step process for generating custom graphs from experimental data.

#### 1. Select Graph Type:

The app currently only supports 3 types of graphs.

- Line graph
- Bar graph
- Scatter plot

The screenshot shows a web form titled "Generate Graph" with a close button (X) in the top right corner. Below the title is a progress bar with five steps: 1. Graph (highlighted with a blue circle), 2. Filter, 3. Parameters, 4. Date, and 5. Customize. Below the progress bar, the text "Type of Graph" is followed by the instruction "Select the graph to display the data". To the right of this text is a dropdown menu labeled "Graph Type \*". At the bottom of the form are two buttons: "Previous" on the left and "Next" on the right.

Figure 16: Highlights the Generate New Graph Button

#### 2. Optional: Apply Filters:

Use this part of the form to filter experiment dates based on a certain attribute. The attribute could be from the Experiment or Raw Data files.

**Note:** Either all form field must be willed out or all must be empty in order to progress to the next stage of the form.

- (a) Choose which data file attribute to filter by
- (b) Choose filter attribute
- (c) Select filter value from dropdown

Generate Graph

Graph Filter Parameters Date Customize

Parameter Type  
Filter with datasheet or experiment attributes

Param Type  
Experiment Log File

Filter Parameters  
Narrow down the data points with an attribute

Filter Attribute  
# of Stacks

Filter Parameters  
Filter by a value

Attribute Value

None  
3  
10  
11

Previous Next

Figure 17: Sample Input of the Filter Step

### 3. Set Parameters:

Select the attributes for the X and Y axis to plot. The two attributes must be from the same experiment sheet.

Generate Graph

Graph Filter Parameters Date Customize

Parameter Type  
Filter with datasheet or experiment attributes

Param Type  
Experiment Log File

Compare Parameters  
Select axis parameters

X\*  
# of Stacks

Y\*  
Potential Diff (V)

Previous Next

Figure 18: Sample Input of the Filter Step

### 4. Selecting Dates:



If no filter is applied, all experiemnt dates will be listed.

Generate Graph

Graph Filter Parameters Date Customize

Experiment Dates  
Select the experimental date(s) of the datasheet(s)

Previous

Select Date \*

- ☒ 2024-02-08
- ☒ 2024-02-09
- ☒ 2024-03-06
- ☐ 2024-03-07

Figure 19: Sample Input of the Date Step

## 5. Customize Display:

Users are able to customize the graphs. All fields on this step are optional. If no axis labels are inputted, the axis would be named the attribute name selected by default.

There are the following options for customization

- Graph title
- Axis Ranges
- Axis Labels

Generate Graph

×

✓

✓

✓

✓

5

Graph

Filter

Parameters

Date

Customize

Graph Title

Title

Custom Axis Settings

Axis Range

Will take min and max values from data set as default

▼

X Axis Range

Set values for the range of the axis

Min

Max

Y Axis Range

Set values for the range of the axis

Min

Max

Axis Labels

▼

X Axis Label

X Axis

Y Axis Label

Y Axis

Previous

Submit

Figure 20: Sample Input of the Filter Step

## 6 Troubleshooting

This section lists common issues, error messages, and their solutions, along with advanced diagnostic procedures.

### 6.1 Common Graphing Issues

Issue	Solution
Dropdown options not appearing	There may be no value for the selected combination of attributes or filters. Check to verify inputted options
Frozen form	There may be a large number of options to select from. Please give the page a few minutes to finishing loading up and displaying all the data
Rendering failed	Validate data selection