

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. We recommend using an Integrated Development Environment (IDE) such as [VS Code](#) for ease of handling the application.

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

These instructions outline the steps to configure a **local** MongoDB database.

- (a) Create a file named `.env` in the root directory of your project.
- (b) Add the following line to the `.env` file:

```
CONNECTION_STRING="mongodb://localhost:27017/"
```

- (c) Save the file.

5. Application Launch

Tip: To switch between directories use the command `cd <directory_name>` to naviagte to a specific directory or `cd ..` to go back one level.

- (a) With `src/backend` as your current directory, start backend:

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

- (b) With `src/frontend` as your current directory, start server:

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

- (c) With `src/frontend` as your current directory, 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. Currently, both Admin and Researcher roles have the same permissions.

Available functionalities 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. This role has limited system configuration capabilities.

Available functionalities include:

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

5 Web Application Pages

5.1 Sign In Process

When users first load the application, they will be greeted by a Sign In screen. If the user has registered credentials, sign in as normal.

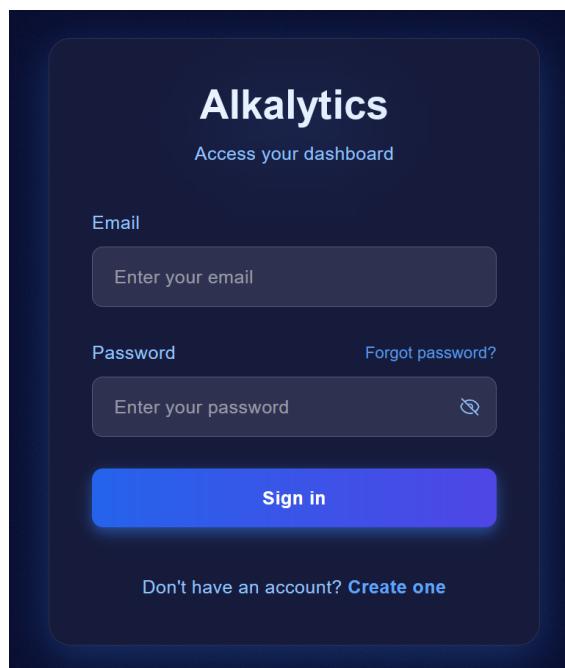


Figure 1: Sign-in Form

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 sign-in form. The user must then enter an email and desired password. There will be two roles to pick from, Researcher and Research Assistant. The admin role is not available for sign up and is only configured by the developer team for the head of the lab. After creating a user account, sign in as normal.

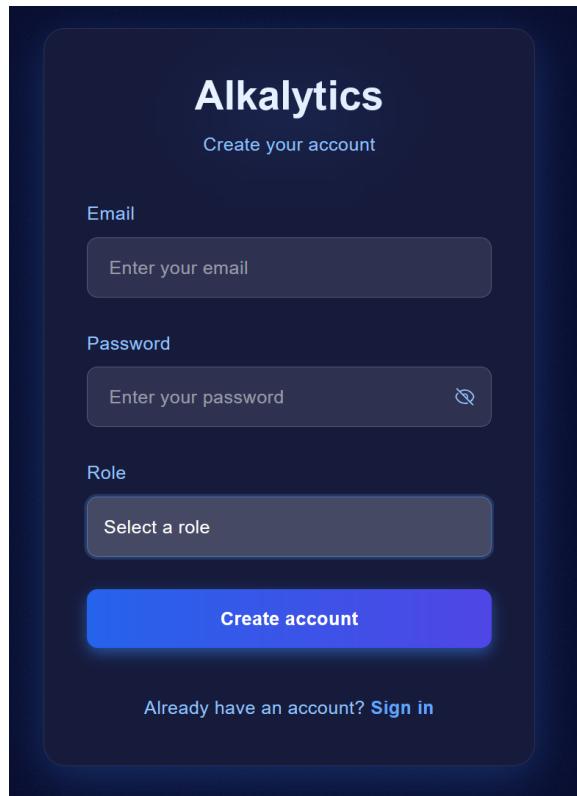


Figure 2: Sign Up Form

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 Interface

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.

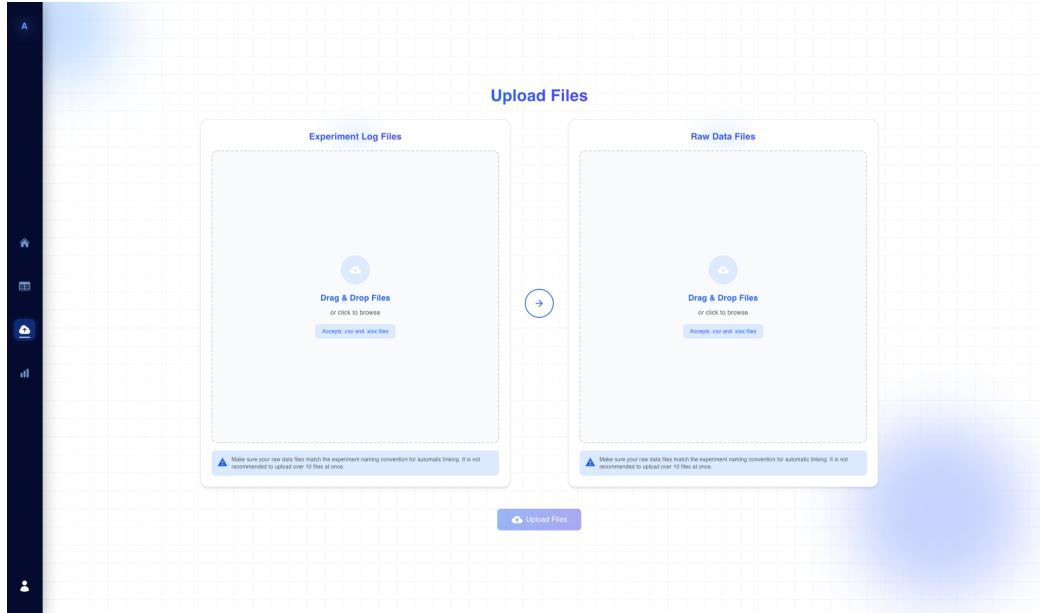


Figure 4: Upload Files Interface

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.

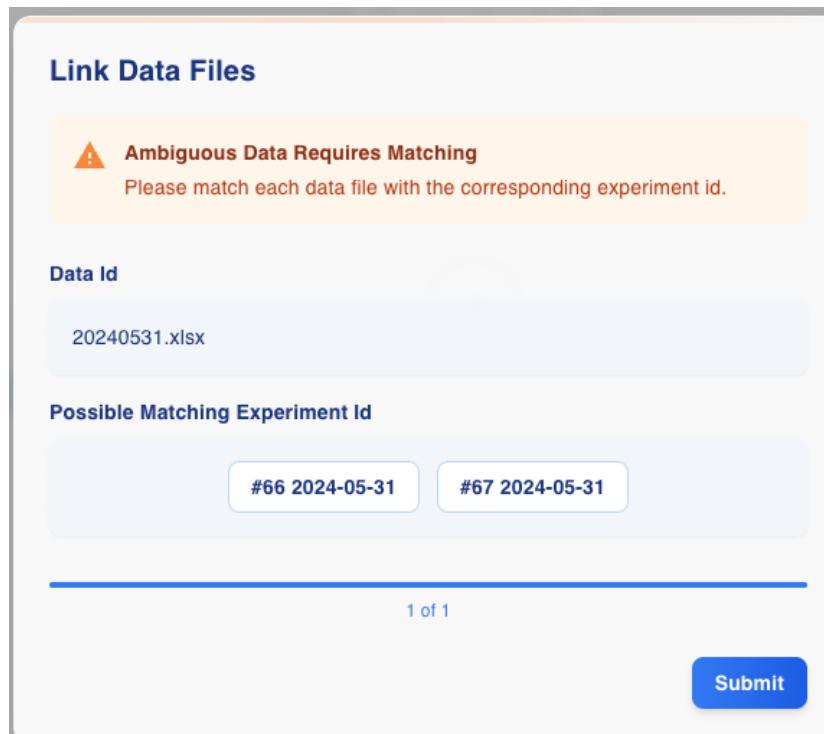


Figure 5: Link Data Files Prompt

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.

The screenshot shows a data table titled "All Experiments". The table has the following columns:

- ID
- EXPERIMENTID
- #
- DATE
- MEMBRANE
- CONFIGURATION
- # OF STACKS
- FLOW RATE (L/H)
- POTENTIAL DIFF (V)
- CURRENT LIMIT (A)
- FEED CONCENTRATION : NACL

The table contains approximately 60 rows of experimental data. Each row includes a checkbox for selection. The rows are numbered from 1 to 60. The data spans from November 2023 to April 2024, covering various membrane types (Membrane, Closed Loop, Continuous) and configurations (Closed Loop, Semi Continuous, FumeTech). Flow rates range from 10 to 50 L/H, potential differences from 5 to 30 V, and current limits from 3 to 10 A.

Figure 6: Experiment Table View

Row Selection The Row Selection feature allows users to select one or more rows for bulk actions such as editing or deleting.

1. Click the checkbox next to each row you wish to select.
2. Perform the desired bulk action (e.g., editing or deleting) on the selected rows.

Edit Dropdown Menu The Edit Dropdown Menu enables users to edit the table directly.

1. Click the "Edit" button to view available options.
2. Select the desired option from the dropdown menu.

Add Column The Add Column feature allows users to introduce a new column into the table for additional data entry.

1. Click the "Add Column" button.
2. Enter a name for the new column in the dialog box that appears.

3. The new column will be added to the right side of the table.

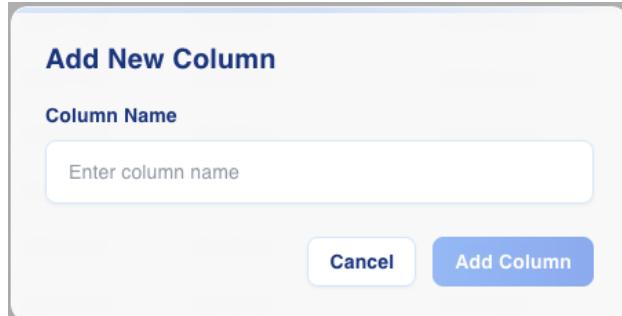


Figure 7: Add New Column Dialog

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 | |
| # <input type="text"/> | |
| # <input type="text"/> | DATE <input type="text"/> yyyy-mm-dd <input type="button" value=""/> |
| MEMBRANE <input type="text"/> | CONFIGURATION <input type="text"/> |
| # OF STACKS <input type="text"/> | FLOW RATE (L/H) <input type="text"/> |
| POTENTIAL DIFF (V) <input type="text"/> | CURRENT LIMIT (A) <input type="text"/> |
| FEED CONCENTRATION NACL <input type="text"/> | FEED CONCENTRATION NAHCO3 <input type="text"/> |
| FEED CONCENTRATION NAOH <input type="text"/> | FEED CONCENTRATION HCL <input type="text"/> |
| FEED CONCENTRATION NA2SO4 <input type="text"/> | FEED CONCENTRATION NAHCO3.1 <input type="text"/> |
| <input type="button" value="Cancel"/> <input type="button" value="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.

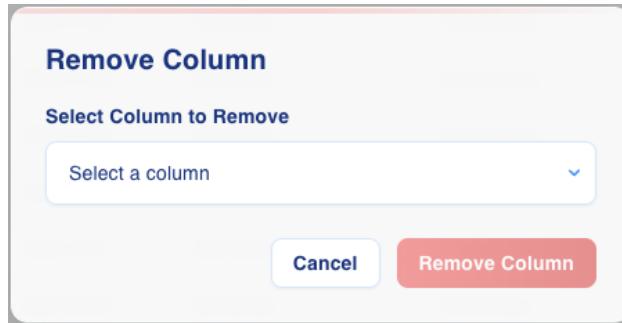


Figure 9: Remove Column Dialog

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.

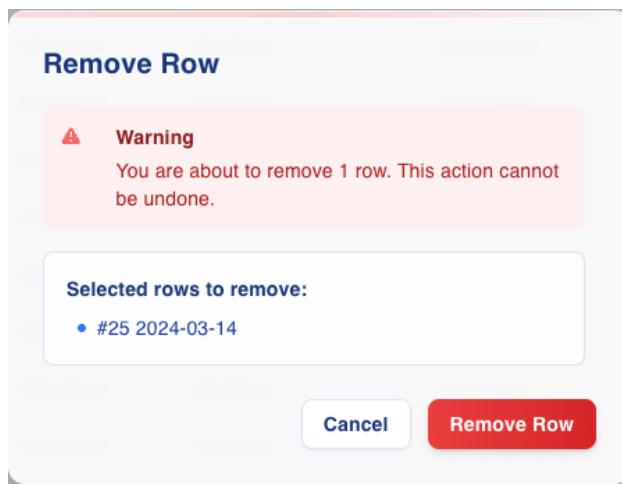


Figure 10: Remove Row Confirmation Dialog

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.

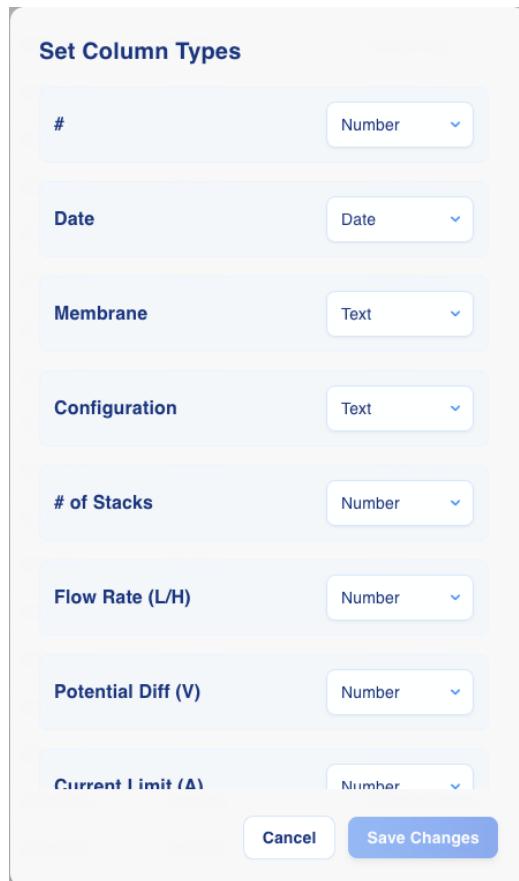


Figure 11: Set Column Types Dialog

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.

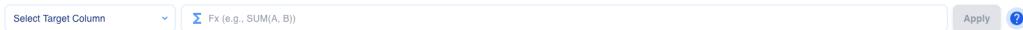


Figure 12: Function Bar

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 η " 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.

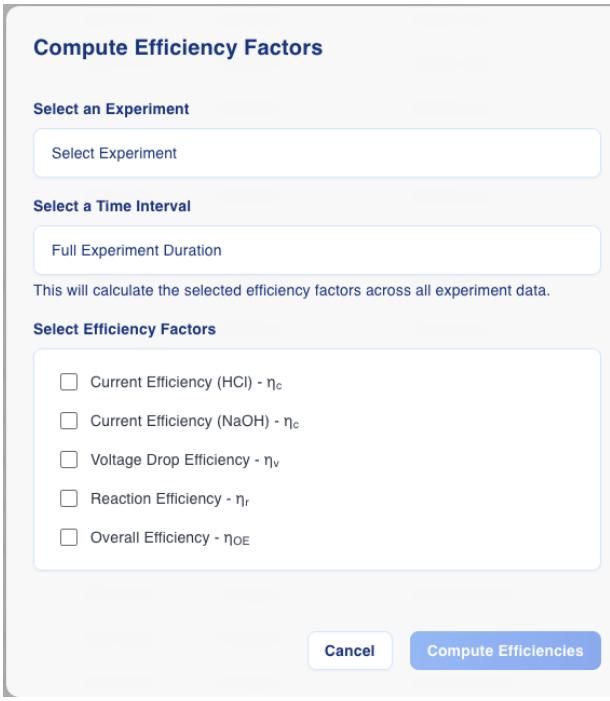


Figure 13: Compute Efficiency Factors Dialog

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.

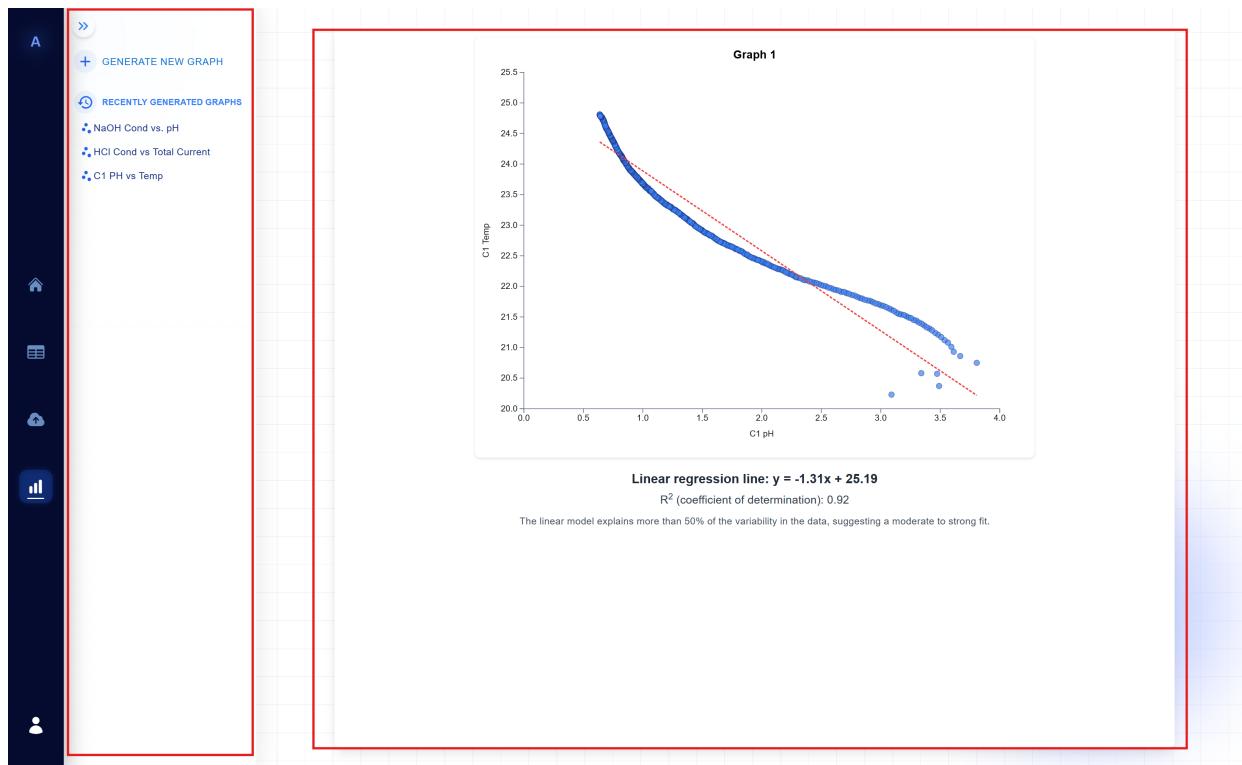


Figure 14: Graph Generation Interface, with Sidebar and Main Content sections highlighted in red

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

Generating a New Graph:

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

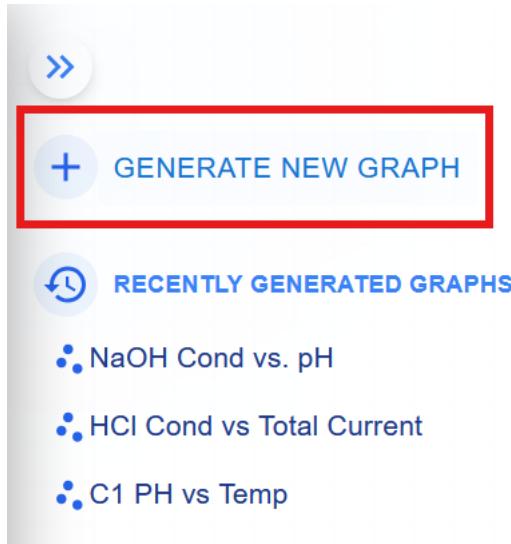


Figure 15: Highlights the Generate New Graph Button

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

Generate Graph

1 2 3 4 5

Graph Filter Parameters Date Customize

Type of Graph
Select the graph to display the data

Graph Type *

Previous Next

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.

- Choose which data file attribute to filter by
- Choose filter attribute
- Select filter value from dropdown

Generate Graph X

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

None
3 10 Next
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 X

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 wil be listed.

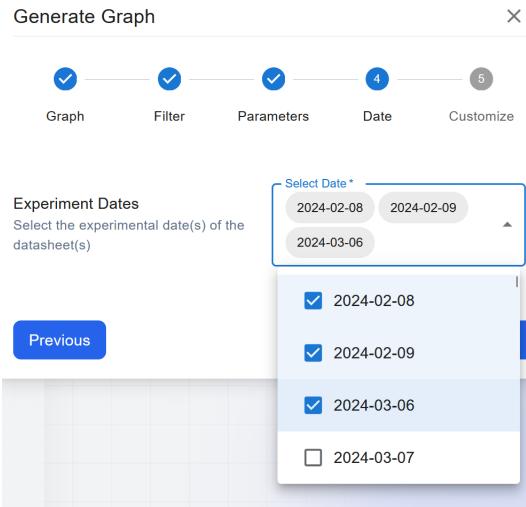


Figure 19: Sample Input of the Date Step

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 nammed the attribute name selected by default.

There are the following options for customization

- Graph title
- Axis Ranges
- Axis Labels

Generate Graph X

Graph Filter Parameters Date Customize

Graph 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

Y Axis Range
Set values for the range of the axis

Axis Labels ▼

X Axis Label

Y Axis Label

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 |