

User Guide for Software Engineering: Alkalytics

Team 21, Alkalytics

Sumanya Gulati

Kate Min

Jennifer Ye

Jason Tran

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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

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

- (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. 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.

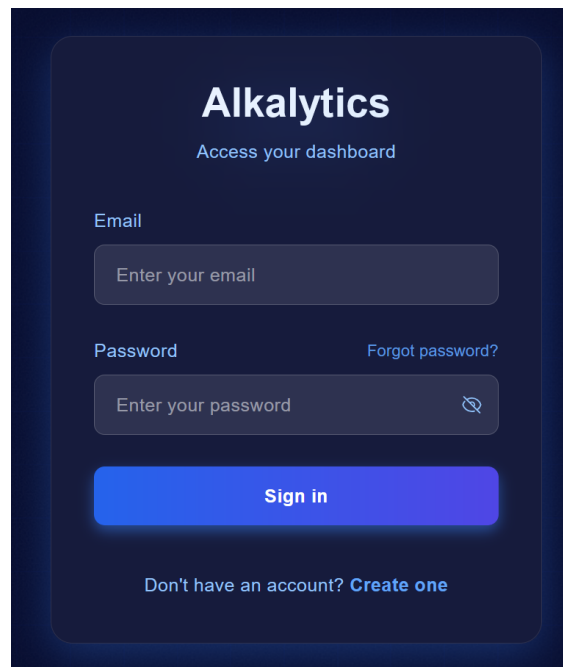
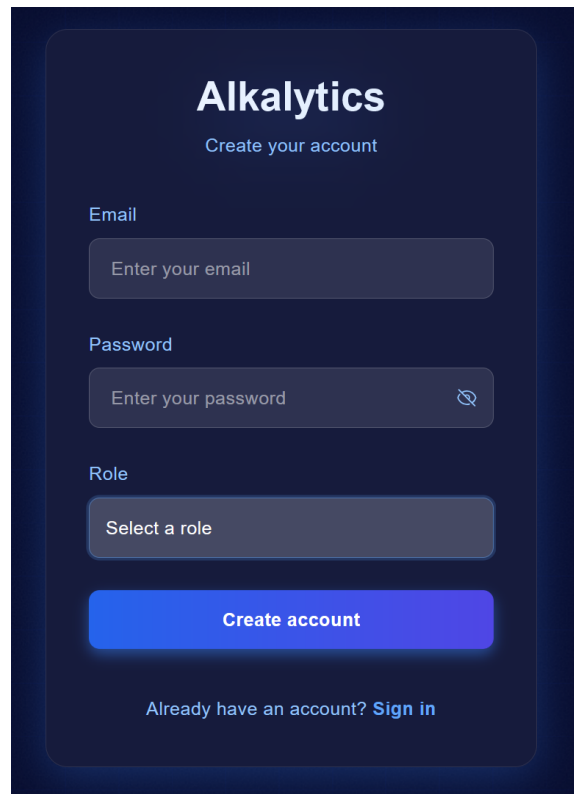
The image shows a sign-in form for 'Alkalytics'. The form is centered on a dark blue background. At the top, the word 'Alkalytics' is written in white, with the tagline 'Access your dashboard' below it. There are two input fields: one for 'Email' with the placeholder text 'Enter your email', and one for 'Password' with the placeholder text 'Enter your password'. To the right of the password field is a link that says 'Forgot password?'. Below the input fields is a large blue button labeled 'Sign in'. At the bottom of the form, there is a link that says 'Don't have an account? Create one'.

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.

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 labeled 'Email', 'Password', and 'Role' with placeholder text 'Enter your email', 'Enter your password', and 'Select a role' respectively, 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 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.

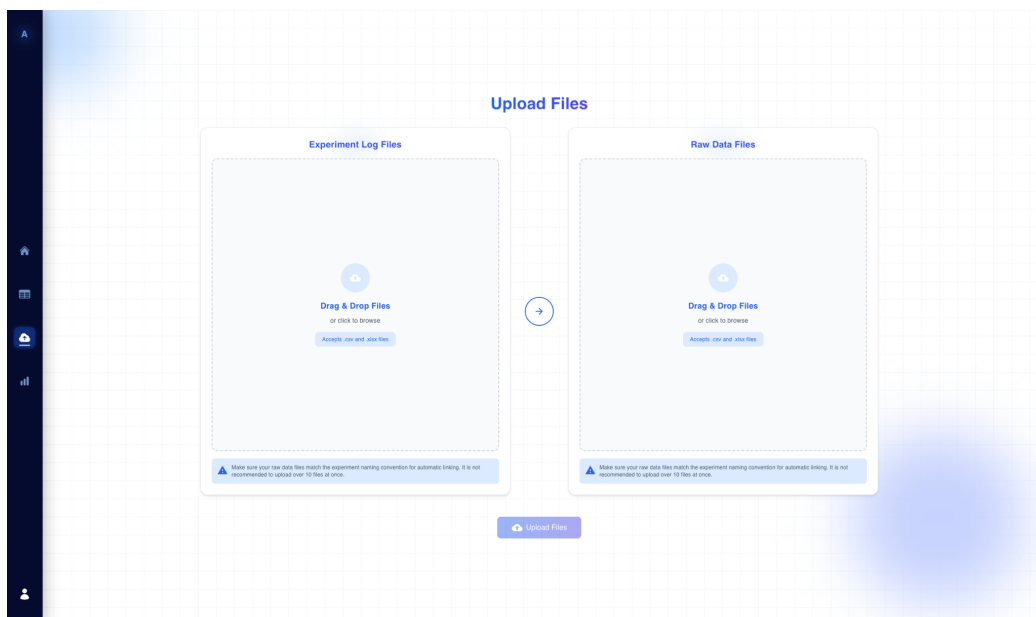


Figure 4: Upload Files Interface

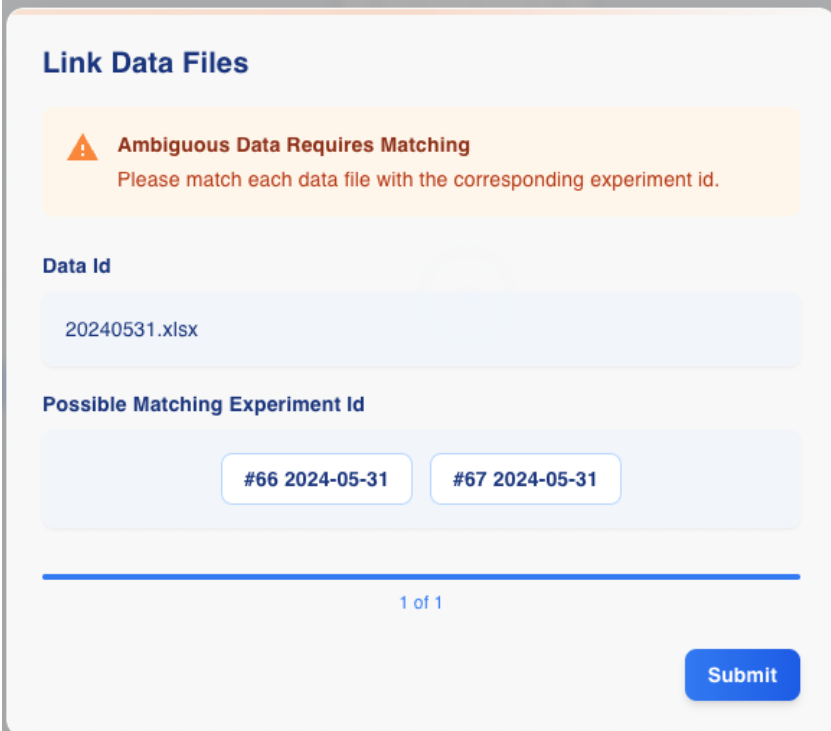
5.4.1 Step-by-Step Upload

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.



The screenshot shows a web interface titled "Link Data Files". At the top, there is a warning message in an orange box: "⚠ Ambiguous Data Requires Matching" followed by "Please match each data file with the corresponding experiment id." Below this, the "Data Id" is displayed as "20240531.xlsx" in a light blue box. Underneath, the "Possible Matching Experiment Id" section shows two selectable options: "#66 2024-05-31" and "#67 2024-05-31", each in its own light blue box. A blue progress bar at the bottom indicates "1 of 1". A blue "Submit" button is located in the bottom right corner.

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.

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

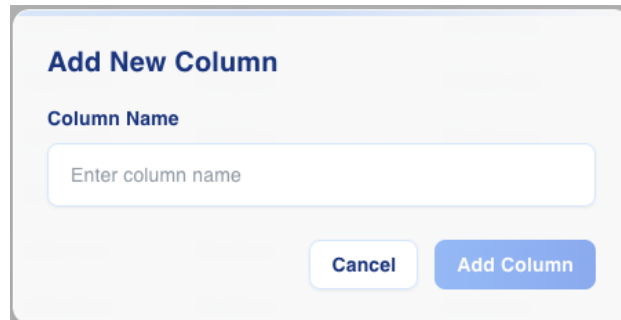
A dialog box titled "Add New Column" with a light gray background and rounded corners. Below the title is the label "Column Name" in a bold, dark blue font. Underneath is a white text input field with a light blue border and the placeholder text "Enter column name". At the bottom right of the dialog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

FEED CONCENTRATION NAHCO₃

FEED CONCENTRATION NAOH

FEED CONCENTRATION HCL

FEED CONCENTRATION NA₂SO₄

FEED CONCENTRATION NAHCO_{3.1}

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.

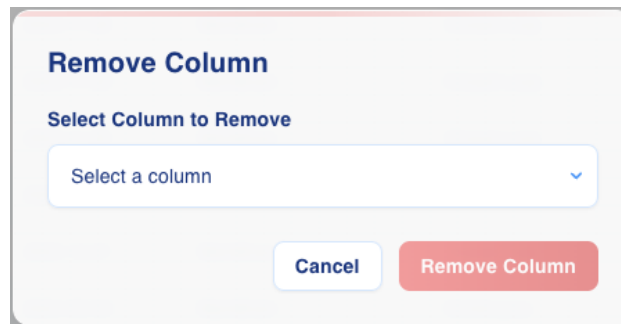


Figure 9: Remove Column Dialog

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.

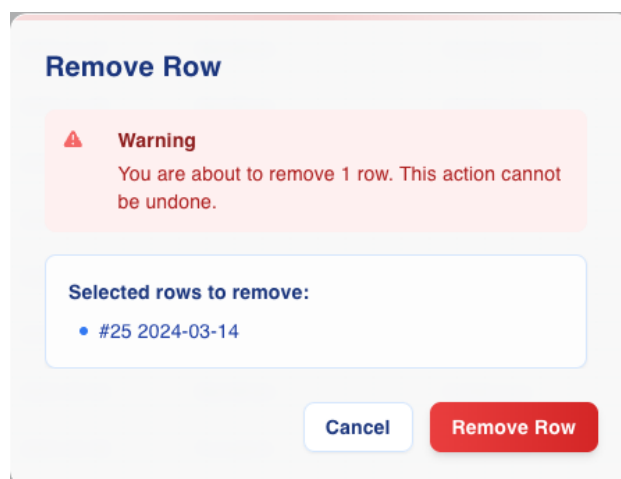
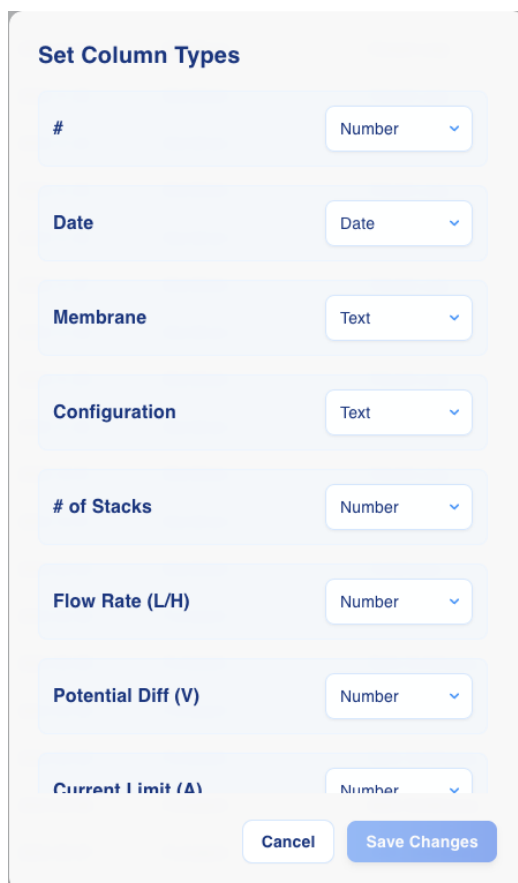


Figure 10: Remove Row Confirmation Dialog

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 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.

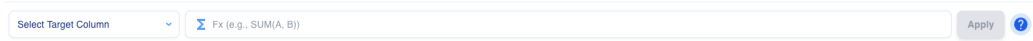
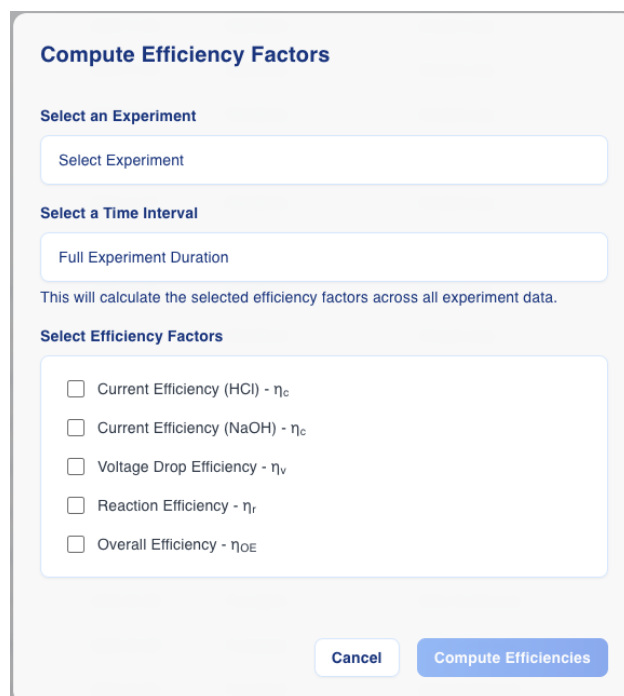


Figure 12: Function Bar

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 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.



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) - η_c
- ☐ Current Efficiency (NaOH) - η_c
- ☐ Voltage Drop Efficiency - η_v
- ☐ Reaction Efficiency - η_r
- ☐ Overall Efficiency - η_{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.

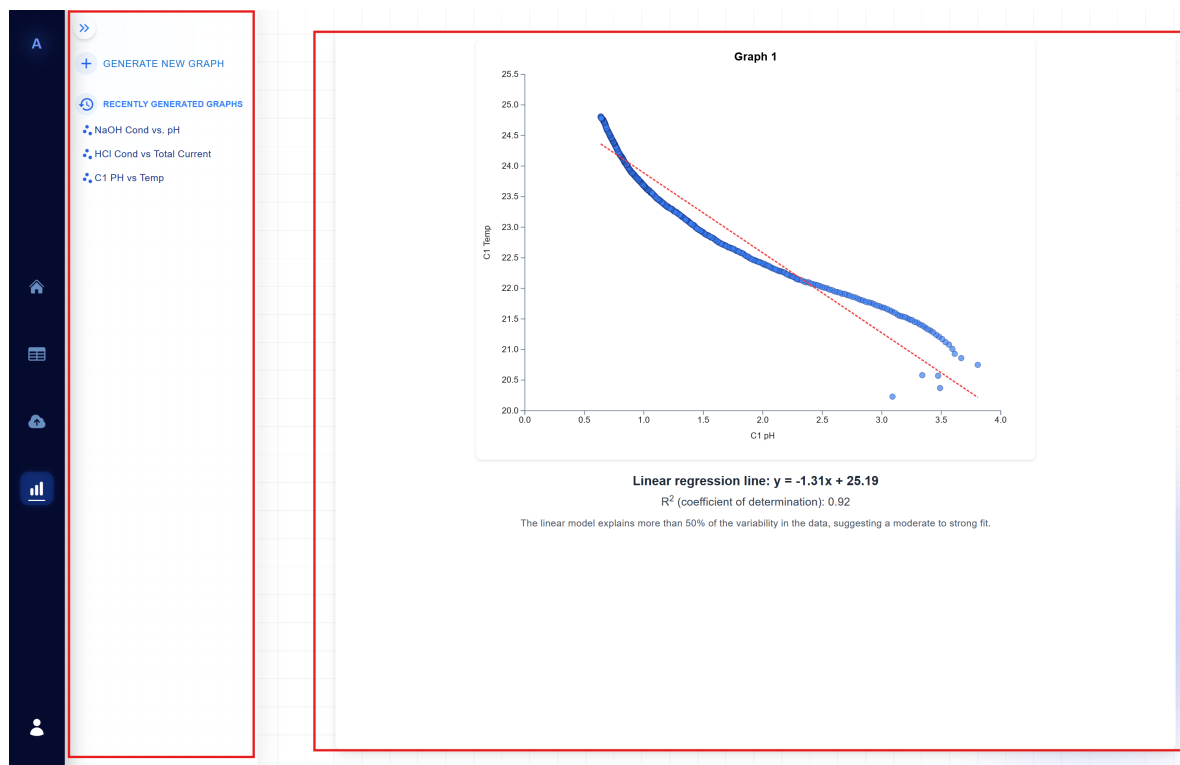


Figure 14: Graph Generation Interface, with Sidebar and Main Content sections highlighted in red

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:

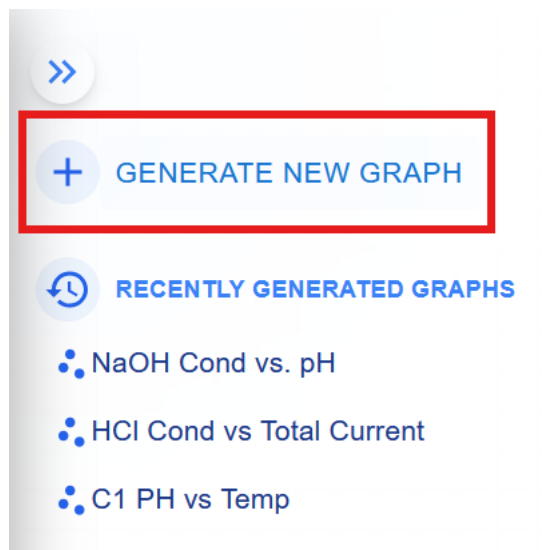


Figure 15: Highlights the Generate New Graph Button

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

The screenshot shows a web form titled "Generate Graph" with a close button (X) in the top right corner. Below the title is a horizontal 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, there is a section labeled "Type of Graph" with the instruction "Select the graph to display the data". To the right of this instruction is a dropdown menu labeled "Graph Type *". At the bottom of the form, there 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 filled 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 |