

User Guide for Software Engineering: Alkalytics

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Contents

1	Introduction	3
2	System Overview	3
2.1	Detailed Requirements	3
3	Installation Guide	3
3.1	Step-by-Step Installation	3
3.2	Verification	4
4	User Management	5
4.1	Admin Features	5
4.2	Researcher Features	5
5	Web Application Pages	5
5.1	Dashboard	5
5.1.1	Key Features	6
5.2	Upload	6
5.2.1	Step-by-Step Upload	7
5.2.2	Linking Raw Data Files to Experiments	7
5.2.3	File Requirements	8
5.2.4	File Upload Types	9
5.2.5	Supported File Formats	9
5.2.6	Upload Guidelines	9
5.3	Data View	10
5.3.1	Common Functionalities	10
5.3.2	Experiment Table	10
5.3.3	Efficiency Table (Read-Only)	17
5.3.4	Raw Data Table (Read-Only)	17
5.4	Graph Generation	18
5.4.1	Detailed Workflow	18
6	Troubleshooting	18

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

This section details the different user roles (Admin and Researcher) and their respective capabilities within the application.

4.1 Admin Features

Administrators have full control over all system functionality including data management, user configuration, and system settings.

4.2 Researcher Features

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

5 Web Application Pages

This section outlines the various pages and functionalities of the web application, such as uploads, processing, and table management.

5.1 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 1: Dashboard Overview

5.1.1 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

5.2 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.

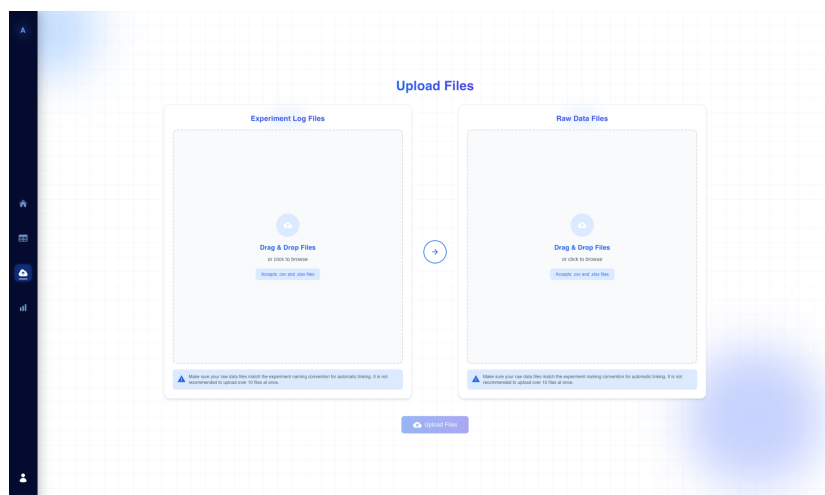


Figure 2: Upload Files Interface

5.2.1 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.

5.2.2 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 3: 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.

5.2.3 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

5.2.4 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.

5.2.5 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.

5.2.6 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.

5.3 Data View

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

5.3.1 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.

5.3.2 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.

Home

Subprocess Data

Experiment Log

Efficiency Calculators

New Entry

Subprocess Data

Experiment Log

Efficiency Calculators

New Entry

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Efficiency Calculators

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Figure 4: 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.

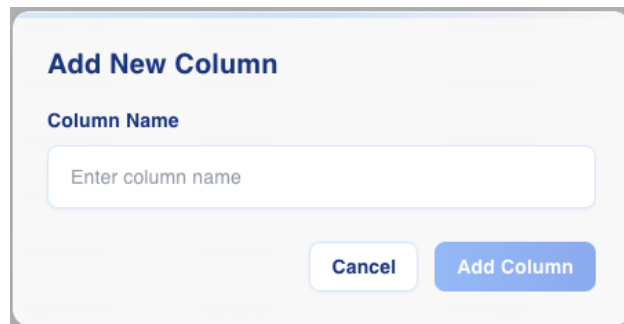
A dialog box titled "Add New Column" with a light gray background and rounded corners. Below the title is the label "Column Name" in a bold, dark blue font. Underneath the label is a white text input field with a light blue border and the placeholder text "Enter column name". At the bottom right of the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

Figure 5: 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 6: 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.

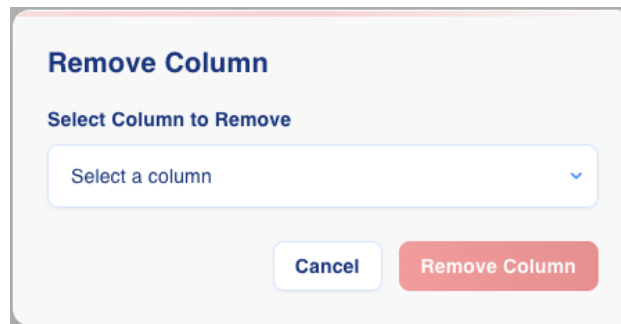


Figure 7: Remove Column Dialog

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.

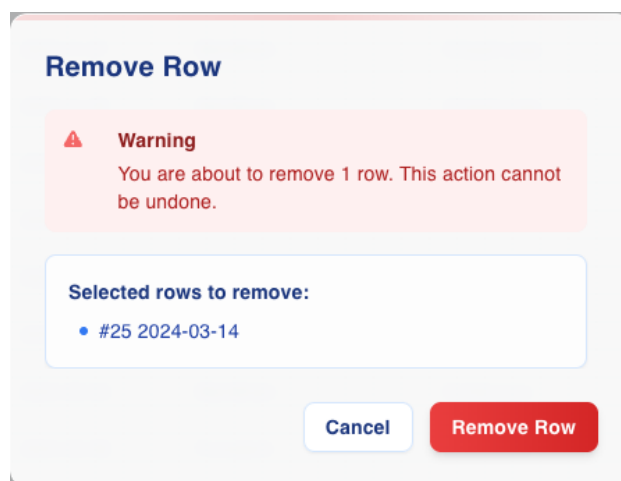


Figure 8: Remove Row Confirmation Dialog

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.

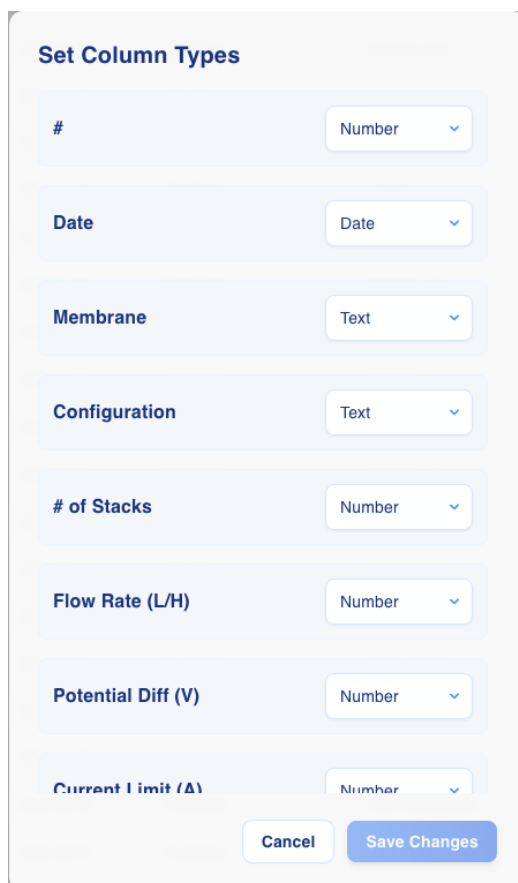
A screenshot of a 'Set Column Types' dialog box. The dialog has a title bar 'Set Column Types' in blue. Below the title, there is a list of columns with their corresponding data types selected in dropdown menus. The columns and their types are: '#' (Number), 'Date' (Date), 'Membrane' (Text), 'Configuration' (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'.

Figure 9: 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.

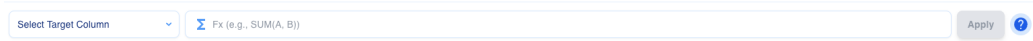


Figure 10: Function Bar

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 11: Compute Efficiency Factors Dialog

5.3.3 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.

5.3.4 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.

5.4 Graph Generation

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

5.4.1 Detailed Workflow

The five-step process for generating custom graphs from experimental data.

1. **Select Graph Type**

- Line graph for trends
- Bar graph for comparisons
- Scatter plot for correlations

2. **Apply Filters**

- (a) Choose filter attribute (e.g., ”# of Stacks”)
- (b) Select filter value from dropdown
- (c) Apply date range if needed

3. **Set Parameters**

- X-axis: Typically time or independent variable
- Y-axis: Measurement or dependent variable

4. **Customize Display**

- Title: Descriptive graph name
- Axis Labels: Clear units of measurement
- Range: Manual or automatic scaling

5. **Generate & Export**

- Click **Submit** to render
- Use **Export** button for PNG/PDF

6 Troubleshooting

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