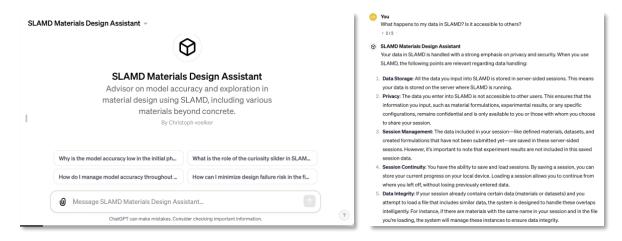
# Try out **SLAMD** Assistant

LINK: https://chat.openai.com/g/g-59lgeS98Q-slamd-assistant



left: SLAMD Assistant User interface; right: Example of a user asking a question about data privacy and security and SLAMD Assistant giving a helpful answer.

The <u>SLAMD Assistant</u> is a specialized AI tool designed to assist users in navigating and utilizing the SLAMD app effectively for cement and concrete research. It provides guidance tailored to the advanced knowledge level of its users, helping them embrace a data-driven approach in their work.

## **Key Functions:**

**Guidance on SLAMD App Usage**: Offers step-by-step assistance on using various features of the SLAMD app, from material selection to experiment setup.

**Problem-Solving and Troubleshooting**: Helps resolve queries and troubleshoot issues encountered while using the SLAMD app.

**Advice on Best Practices**: Provides recommendations on best practices for efficient use of the SLAMD app's functionalities.

## **Usage Tips:**

- Ask direct questions about specific SLAMD app features or processes.
- Seek assistance for any difficulties faced during the app's usage.
- Request recommendations for optimizing the use of the app in your projects.

The SLAMD Assistant communicates in a straightforward, user-friendly manner, ensuring clarity and ease of understanding. Its focus is on helping users get started and efficiently guiding them through their development journey with the SLAMD app.

# **User Manual**

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- 7. Material Discovery
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### 1. Overview

This document describes how to use the SLAMD app. The various screenshots below contain various test data and are not meant to demonstrate actual use cases.

The general workflow of the app is as follows:

- 1. Define basic materials and processes
- 2. Use basic materials to create combined materials by blending them
- 3. Use all defined materials to create formulations, which make up a dataset
- 4. Enrich a dataset with targets (labels) if necessary
- 5. Predict properties of the materials in a dataset for use in Sequential Learning

In addition to this workflow, SLAMD includes a Design Assistant module. On the one hand it allows for the creation of materials in a chat-based environment fashion. On the other hand it integrated LLMs for generating new promising formulations.

# 2. Navigation Bar

The navigation bar contains the following elements:

- A "burger menu" that opens a sidebar with similar functionality, mostly for smaller devices
- A "Home" button, which leads to the landing page that is first shown after opening the app
- A "Design Assistant" button, which leads to the design assistant page (See "2. Design Assistant")
- A "Base" button, that leads to the base materials page (See "4. Base Materials and Processes")
- A "Blend" button, that leads to the material blending page (See "5. Blended Materials")
- A "Formulations" button, that leads to the Formulations page (See "6. Material Formulations")

- A "Discovery" button, that leads to the Discovery page (See "7. Material Discovery")
- A "Save" button (downwards pointing arrow)
  - Pressing the save button allows you to save your current session to your local device
  - This includes all defined materials, all datasets and all created formulations that have not been submitted yet. Further, it saves the current state of the design assistant, i.e. the conversation.
  - This does not include experiment results
- A "Load" button (upwards pointing arrow)
  - Pressing the load button allows you to load a session that you have previously saved to your device
  - Your current session will not be deleted
  - o If your session already contains materials or chats included in the file, the versions in the file will not be ignored. Rmk: This uses internal IDs that need to match; there can be multiple materials with the same name
  - If your session already contains datasets included in the file, the datasets will still be uploaded but renamed
- A "Clear" button (trash can)
  - o Pressing the clear button will delete all data in your current session
  - You will be asked for confirmation when pressing the button
  - Make sure to back up your work
- A "Manual" button (question mark)
  - o Provides a link to this manual

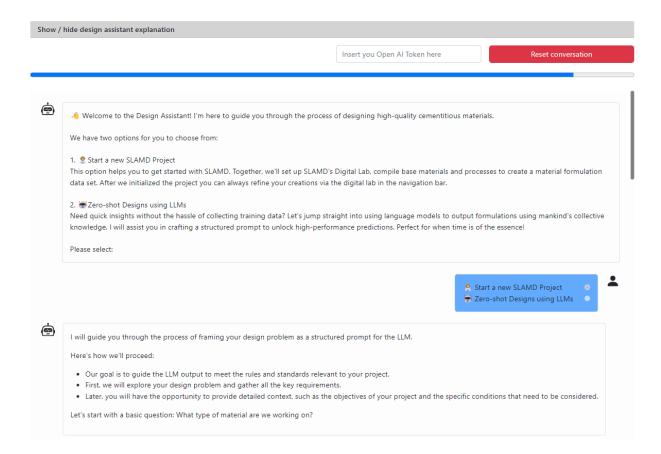


## 3. Design Assistant

The design assistant can be used for two purposes:

- 1) New Project: It guides the user towards creating materials in natural language
- 2) Zero-shot Assistant: By using the power if LLMs, new promising recipes can be generated in a chat-based fashion.

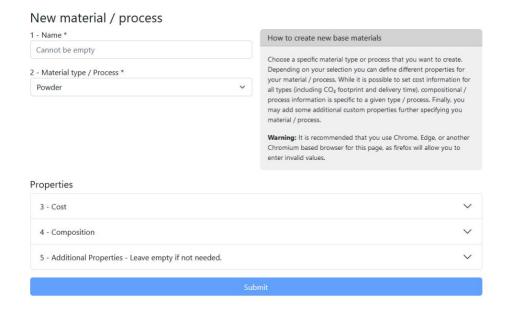
Using the assistant is straightforward. As a chatbot, it guides the user step-by-step in both scenarios. Note that the zero-shot setup is ground in generative AI. While the potential for applying LLMs to such a use case was verified in scientific papers, the user should still view this functionality as experimental.



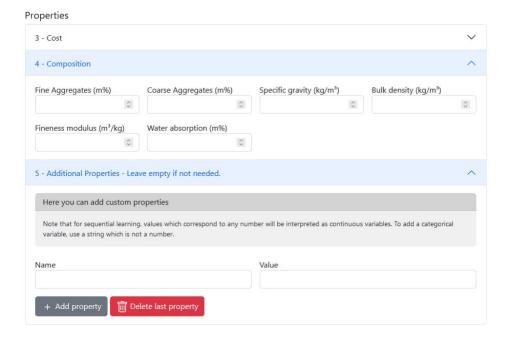
## 4. Base Materials and Processes

The first step of the non-chat workflow is the creation of base materials and processes. First, choose a name for your new material. Then select its type from the dropdown.

There are six different types: Powder, Liquid, Aggregates, Admixture, Process, and Custom. These types differ in which kinds of attributes they have and how they are treated on the formulations page.



Every type has Cost properties. Most other types also have additional properties depending on their type. The Custom type is special: It does not have any predefined properties outside of Cost, and relies on custom properties to carry information. All types can also hold custom "Additional Properties".



Depending on the property inputs may be alphanumerical (numbers, letters, and certain symbols) or limited to numbers (numbers and decimal separators only). Note that most browsers will prevent you from entering invalid values, **with the exception of firefox.** If you enter an invalid value it is automatically dropped.

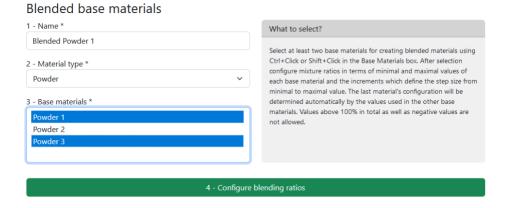
There may be at most 10 "Additional" properties and their type is automatically determined. If you enter a number it will be interpreted as a continuous variable. If you enter anything else it will be interpreted as a categorical variable. Make sure to format your input correctly. You may use either "." or "," as decimal separator. Finally, Additional Properties also require entering a property name.

Any property may be left empty. Note that for later creation of blended materials in the next step a base material with at least one field empty (in costs or composition) is considered incomplete and a warning will be shown on the blend page. However, blending can still be performed. If you want Additional Properties to be blended correctly their name must match exactly on all materials involved.

Once you have finished editing your material you may save it by clicking the "Submit" button. It will then appear in the table below. You may delete it by clicking the red trash can button, or load it for editing by clicking the grey pen button.

#### 5. Blended Materials

Next you may create blended materials. Select a name, a type, and at least two starting materials. You can select multiple materials by using Ctrl+Click or Shift+Click.



Blended materials are mixtures of their base materials. The properties of these blended materials are given by the respective properties of the base materials, using the composition as weights.

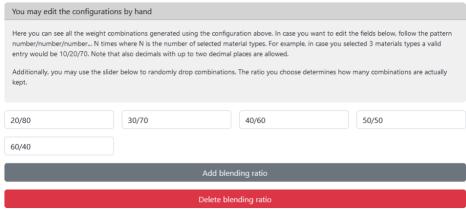
For example, if you have two powders both solely described by "Specific gravity" you can define a blend e.g. of 10% the first powder and 90% the second one. The resulting Specific gravity is then computed as the weighted sum of the original Specific gravities: specific\_gravity\_combined =  $0.1 * \text{specific_gravity}_1 + 0.9 * \text{specific_gravity}_2$ .

The same logic applies to all the other properties except for "Delivery time" which is defined as the maximum of the base materials Delivery times.

Using the "Increment" input multiple combinations can be created at once. In the example below, blended materials with ratios 20/80, 30/70, 40/60, 50/50 and 60/40 will be created. The amount of the last base material is automatically calculated from the other materials to fill 100%.

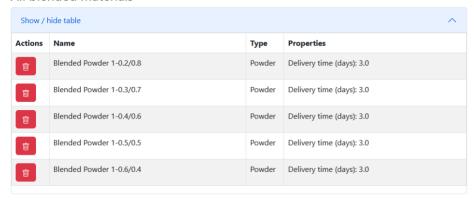


Press the "Preview blending ratios" button to continue. In the preview you can see all the combinations that will be created. You may also adjust the weights here if you wish. Using the "Add blending ratio" you can also add entirely new ratios. If you enter numbers that do not add up to 100 they will automatically be normalized.



Finally, once you are finished configuring the blended material, click the "Submit" button to create your blends. The created entries are saved and displayed in a table at the bottom of the page. You may delete created blended materials using the red trashcan buttons.

#### All blended materials



In case one or all of the base materials do not have all of their properties specified the blend material page will show a box with an "Incomplete Data" warning. In this case you need to be aware of some additional rules.

#### Incomplete data

The chosen configuration is not complete! Check that all properties are specified among all chosen base materials. Further, make sure that all additional properties have the same keys and matching data types for a given key. If you nevertheless want to continue with the chosen setup, not all blended properties will be inferred.

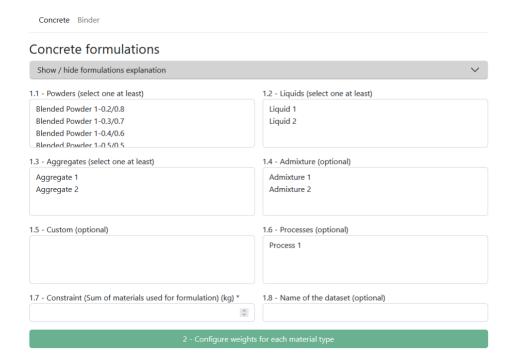
Assume you want to mix two base materials which both define a structural property called 'Base Material Property' and assume both define an additional property called 'Add. Prop'. Then there are several possible cases:

- Base Material Property is filled for all base materials → the resulting blended materials have the property Base Material Property computed as the weighted sum of its base materials' Base Material Property values
- At least one of the base materials did not specify a value for Base Material Property → the resulting blend will not have the property either as the description is not complete
- Add. Prop is filled for all base materials and has only numeric values → the resulting blended materials have the property Add. Prop computed as the weighted sum of their base materials Add. Prop values
- Add. Prop is filled for all base materials and only has non-numeric values → the resulting blended materials will have a property for each value of Add. Prop. For example, if Add. Prop had value X for the first material and value Y for the second material, the blended material will have two properties X and Y, but no property "Add. Prop". The values of X and Y are then given by the blending ratios of the respective base materials.
- Add. Prop is filled for all base materials and some have non-numeric values while for others the values are numeric → Incomplete description: no corresponding additional property is created for the blended materials

## 6. Material Formulations

Now that the materials are defined, a dataset needs to be built for predictions. Datasets are built from formulations.

A formulation combines materials and processes. The app currently supports Concrete formulations and Binder formulations. A concrete formulation needs to contain a powder, a liquid, and an aggregate. A binder formulation needs to contain a powder and a liquid. Additional materials and processes may be added freely.

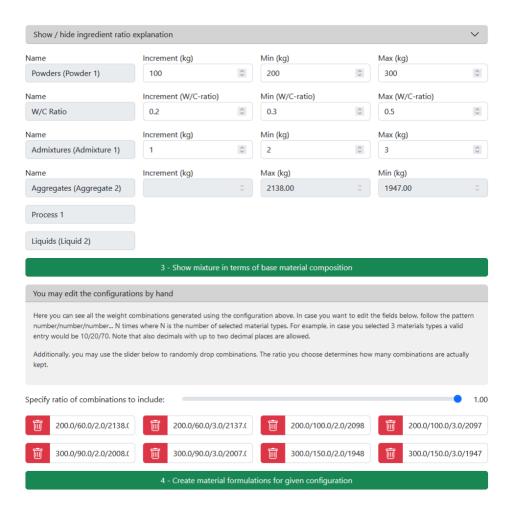


In addition to the selected materials and processes you need to define a weight constraint. This corresponds to the total weight of the mix of materials to be used for the formulation. Further, you can optionally specify a name for the dataset.

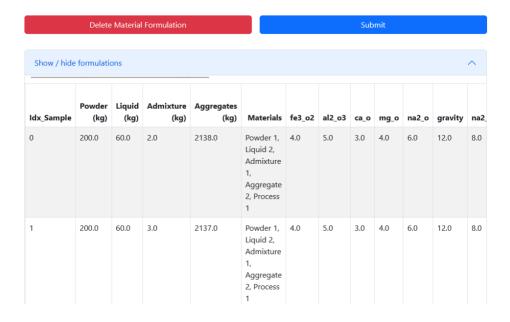
Click the "Configure weights for each material type" button to configure the ratios of the chosen materials. This works similar to the blend materials page. However, there are some key differences:

- The form autocompletes not to 100%, but the chosen constraint
- Liquids are not specified directly, but using the W/C ratio, relative to the Powder value. For example, for 200kg Powder and 0.5 Liquid, there will be 100kg Liquid. See also the ingredient ratio explanation infobox.

Click the "Show mixture in terms of base material composition" button to see all newly generated material configurations. As on the blend page, you may edit these by hand. You may additionally randomly drop some of these configurations using the slider. In case you generated too many combinations you may select a fraction of configurations that you want to keep. They will be selected randomly from the full set.



Finally, click the "Create material formulations for given configuration" button to create a new batch of samples. They will be shown at the bottom of the page.



You may now repeat the process to add more samples, or press the "Submit" button to save these formulations as a dataset. If you specified a name at the beginning, this name will be used; otherwise, a name will be automatically generated. Note that you can leave the page and return later without losing your formulations, although you will have to re-enter the dataset name if you wish to submit it.

You can also clear all created formulations by pressing the "Delete Material Formulation" button.

After you have saved, the dataset can be found on the discovery page.

## 7. Material Discovery

On the discovery page all your previously created datasets are shown. You can also upload new datasets directly using CSV files (with utf-8 encoding).



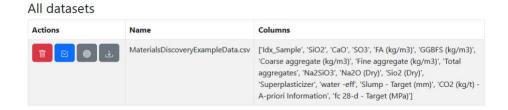
Make sure you properly format your CSV file. Allowed formats are

- column separator: "," and decimal delimiter "."
- column separator: ";" and decimal delimiter ","

For example, two valid CSV files with only two columns and one row would look like this:

```
col1,col2
1.2,2.1
or
col1;col2
1,2;2,1
```

After successful upload the file is shown in a table:



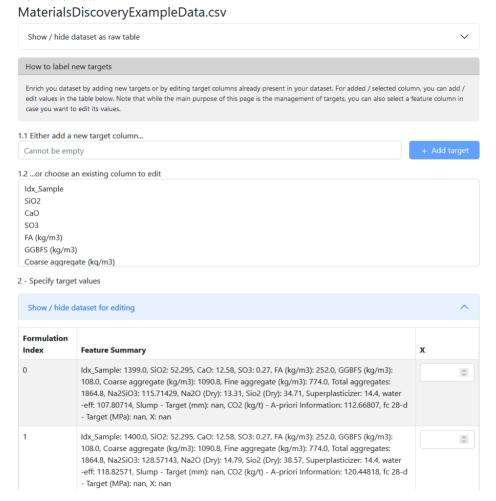
There are several actions available for each dataset:

- Delete (red trash can button)
- Select for running an experiment (blue checkmark button)
- Modify targets (grey "bullseye" button, see below)
- Download (grey downward arrow button)

#### 7.1 Specify Targets

The targets page allows you to add new columns to a dataset or modify existing ones. Its purpose is to enter new experimental data, but in a pinch it can also be used to edit a dataset. It is reached by pressing the grey "bullseye" button next to a dataset on the Discovery page.

On top of the page is an infobox that allows you to view the entire dataset as a formatted table. Below, there are elements that allow you to specify target values. Either type a label into the textbox and press the "Add target" button to add a column, or select one of the existing columns from the list.



Either way the chosen target is added to the table at the bottom, with input fields that allow you to input values for each row. If you chose a row with existing data, these input fields may be prefilled. Modify these columns as you wish, then press the "Save targets" button at the bottom of the page to save your changes and return to the Discovery page.

#### 7.2 Configuring and runing an experiment

Once you have prepared a dataset to your liking it can be used for an experiment. Start by selecting it with the blue checkmark button next to its entry in the dataset table.

First, select the input columns that you want to use. These are called the features. Any column can be used as a feature, but columns containing missing data will be dropped before training. Remember that you can select multiple entries individually using Ctrl+Click, or select many entries at once using Shift+Click.

Once you have selected some features the remaining columns can be chosen as targets in a similar way. Target columns must be partially labelled to provide training data (at least 1 label for Gauss, at least 2 labels for Random Forest). They may not be fully labelled or fully unlabelled. If you select multiple targets, the rows for which the different targets are labelled do not need to match. However, the novelty can only be calculated if there are fully labelled rows.

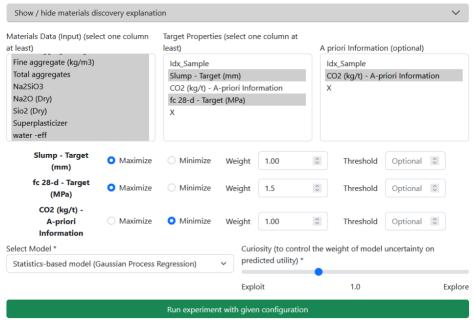
Columns that are used neither as features nor as targets may be used as a priori information. A priori information is used in the utility calculation, but is not predicted.

For each chosen target and a priori information you may now select how it affects the utility calculation.

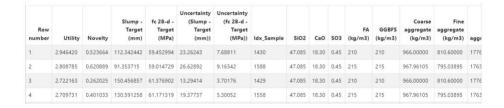
- You may select whether to minimize (lower values correspond to higher utility) or maximize (higher values correspond to higher utility)
- You may select a weight (for a weight of e.g. 1.2, the impact on utility is 20% larger)
- You may select a threshold, which can have different effects depending on whether you are working with a target or an a priori property:
  - Minimizing a target with threshold T: Target predictions are not affected. However, all predicted target values smaller or equal than T contribute to the utility equally
  - Maximizing a target with threshold T: Target predictions are not affected.
     However, all predicted target values bigger or equal than T contribute to the utility equally
  - Minimizing an a-priori information with threshold T: All rows with values for the chosen a-priori information above T are simply dropped → no predictions are made for these rows
  - Maximizing an a-priori information with threshold T: All rows with values for the chosen a-priori information beelow T are simply dropped → no predictions are made for these rows

Finally, you can select a prediction model and a curiosity. The latter influences how uncertainty is used in the utility calculation. For higher curiosity, uncertainty is weighted higher, which prefers unknown regions of the parameter space. For low values this effect is lessened. For negative values uncertainty is used as a penalty, preferring known regions of the parameter

#### space.



Once you have configured the experiment, run it by pressing the "Run experiment with given configuration" button. The results are shown in a table at the bottom of the page. It is sorted by utility such that the first row represents the most promising candidate with respect to the parameters you have chosen in the form above.



You can inspect the predictions more closely using plots which show the predicted targets and utility. Hovering over the point shows information about the given point. Further you can request a tSNE plot representation of the dataset by expanding the matching element. Additionally, there is a button for downloading the prediction data. An excel file is created containing sheets for the predicted data, the original data and the configuration that was used for making the prediction.

