

User Manual

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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.

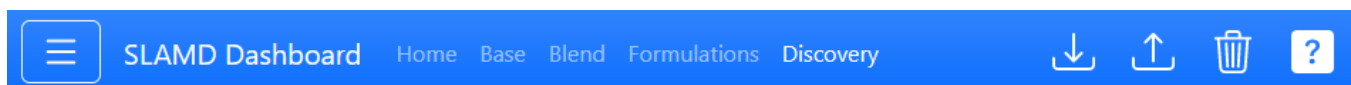
The general workflow of the app is as follows:

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

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 "Base" button, that leads to the base materials page (See "3. Base Materials and Processes")
- A "Blend" button, that leads to the material blending page (See "4. Blended Materials")
- A "Formulations" button, that leads to the Formulations page (See "5. Material Formulations")
- A "Discovery" button, that leads to the Discovery page (See "6. 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
 - 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
 - If your session already contains materials included in the file, the versions in the file will not be ignored. 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)
 - 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)
 - Provides a link to this manual



3. Base Materials and Processes

The first step of the 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.

New material / process

1 - Name *

Cannot be empty

2 - Material type / Process *

Powder



How to create new base materials

Choose a specific material type or process that you want to create. Depending on your selection you can define different properties for your material / process. While it is possible to set cost information for all types (including CO₂ footprint and delivery time), compositional / process information is specific to a given type / process. Finally, you may add some additional custom properties further specifying you material / process.

Warning: It is recommended that you use Chrome, Edge, or another Chromium based browser for this page, as firefox will allow you to enter invalid values.

Properties

3 - Cost



4 - Composition




5 - Additional Properties - Leave empty if not needed.




Submit

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".

Properties

3 - Cost 

4 - Composition 

Fine Aggregates (m%)


Coarse Aggregates (m%)

Specific gravity (kg/m³)

Bulk density (kg/m³)

Fineness modulus (m³/kg)

Water absorption (m%)

5 - Additional Properties - Leave empty if not needed. 


Here you can add custom properties

Note that for sequential learning, values which correspond to any number will be interpreted as continuous variables. To add a categorical variable, use a string which is not a number.

Name

Value

+ Add property

 Delete last property

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.

4. 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 base materials

1 - Name *

Blended Powder 1

2 - Material type *

Powder

3 - Base materials *

Powder 1

Powder 2

Powder 3

What to select?

Select at least two base materials for creating blended materials using Ctrl+Click or Shift+Click in the Base Materials box. After selection configure mixture ratios in terms of minimal and maximal values of each base material and the increments which define the step size from minimal to maximal value. The last material's configuration will be determined automatically by the values used in the other base materials. Values above 100% in total as well as negative values are not allowed.

4 - Configure blending ratios

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: $specific_gravity_combined = 0.1 * specific_gravity_1 + 0.9 * specific_gravity_2$.

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%.

Name	Increment (%)	Min (%)	Max (%)
Powder 1	10	20	60

Name	Increment (%)	Max (%)	Min (%)
Powder 3		80.00	40.00

5 - Preview blending ratios

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.

You may edit the configurations by hand

Here you can see all the weight combinations generated using the configuration above. In case you want to edit the fields below, follow the pattern number/number/number... N times where N is the number of selected material types. For example, in case you selected 3 materials types a valid entry would be 10/20/70. Note that also decimals with up to two decimal places are allowed.






Additionally, you may use the slider below to randomly drop combinations. The ratio you choose determines how many combinations are actually kept.

Add blending ratio

Delete blending ratio

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

Show / hide table ^			
Actions	Name	Type	Properties
	Blended Powder 1-0.2/0.8	Powder	Delivery time (days): 3.0
	Blended Powder 1-0.3/0.7	Powder	Delivery time (days): 3.0
	Blended Powder 1-0.4/0.6	Powder	Delivery time (days): 3.0
	Blended Powder 1-0.5/0.5	Powder	Delivery time (days): 3.0
	Blended Powder 1-0.6/0.4	Powder	Delivery time (days): 3.0

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

5. 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.

Concrete Binder

Concrete formulations

Show / hide formulations explanation



1.1 - Powders (select one at least)

Blended Powder 1-0.2/0.8
Blended Powder 1-0.3/0.7
Blended Powder 1-0.4/0.6
Blended Powder 1-0.5/0.5

1.2 - Liquids (select one at least)

Liquid 1
Liquid 2

1.3 - Aggregates (select one at least)

Aggregate 1
Aggregate 2

1.4 - Admixture (optional)

Admixture 1
Admixture 2

1.5 - Custom (optional)

1.6 - Processes (optional)

Process 1

1.7 - Constraint (Sum of materials used for formulation) (kg) *

1.8 - Name of the dataset (optional)

2 - Configure weights for each material type

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.

Show / hide ingredient ratio explanation



Name	Increment (kg)	Min (kg)	Max (kg)
Powders (Powder 1)	<input type="text" value="100"/>	<input type="text" value="200"/>	<input type="text" value="300"/>

Name	Increment (W/C-ratio)	Min (W/C-ratio)	Max (W/C-ratio)
W/C Ratio	<input type="text" value="0.2"/>	<input type="text" value="0.3"/>	<input type="text" value="0.5"/>

Name	Increment (kg)	Min (kg)	Max (kg)
Admixtures (Admixture 1)	<input type="text" value="1"/>	<input type="text" value="2"/>	<input type="text" value="3"/>

Name	Increment (kg)	Max (kg)	Min (kg)
Aggregates (Aggregate 2)	<input type="text"/>	<input type="text" value="2138.00"/>	<input type="text" value="1947.00"/>

Process 1

Liquids (Liquid 2)

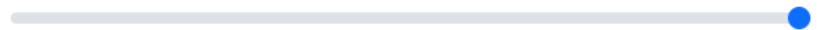
3 - Show mixture in terms of base material composition

You may edit the configurations by hand

Here you can see all the weight combinations generated using the configuration above. In case you want to edit the fields below, follow the pattern number/number/number... N times where N is the number of selected material types. For example, in case you selected 3 materials types a valid entry would be 10/20/70. Note that also decimals with up to two decimal places are allowed.

Additionally, you may use the slider below to randomly drop combinations. The ratio you choose determines how many combinations are actually kept.

Specify ratio of combinations to include:



1.00

200.0/60.0/2.0/2138.0	200.0/60.0/3.0/2137.0	200.0/100.0/2.0/2098	200.0/100.0/3.0/2097
300.0/90.0/2.0/2008.0	300.0/90.0/3.0/2007.0	300.0/150.0/2.0/1948	300.0/150.0/3.0/1947

4 - Create material formulations for given configuration

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.

Delete Material Formulation

Submit

Show / hide formulations



Idx_Sample	Powder (kg)	Liquid (kg)	Admixture (kg)	Aggregates (kg)	Materials	fe3_o2	al2_o3	ca_o	mg_o	na2_o	gravity	na2_o
0	200.0	60.0	2.0	2138.0	Powder 1, Liquid 2, Admixture 1, Aggregate 2, Process 1	4.0	5.0	3.0	4.0	6.0	12.0	8.0
1	200.0	60.0	3.0	2137.0	Powder 1, Liquid 2, Admixture 1, Aggregate 2, Process 1	4.0	5.0	3.0	4.0	6.0	12.0	8.0

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.

6. 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).

Material Discovery

CSV File Upload

Durchsuchen...

Keine Datei ausgewählt.



Upload dataset

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:

All datasets

Actions	Name	Columns
   	MaterialsDiscoveryExampleData.csv	['Idx_Sample', 'SiO2', 'CaO', 'SO3', 'FA (kg/m3)', 'GGBFS (kg/m3)', 'Coarse aggregate (kg/m3)', 'Fine aggregate (kg/m3)', 'Total aggregates', 'Na2SiO3', 'Na2O (Dry)', 'Sio2 (Dry)', 'Superplasticizer', 'water -eff', 'Slump - Target (mm)', 'CO2 (kg/t) - A-priori Information', 'fc 28-d - Target (MPa)']

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)

6.1 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.

MaterialsDiscoveryExampleData.csv

Show / hide dataset as raw table

How to label new targets

Enrich you dataset by adding new targets or by editing target columns already present in your dataset. For added / selected column, you can add / edit values in the table below. Note that while the main purpose of this page is the management of targets, you can also select a feature column in case you want to edit its values.

1.1 Either add a new target column...

Cannot be empty

+ Add target

1.2 ...or choose an existing column to edit

- Idx_Sample
- SiO2
- CaO
- SO3
- FA (kg/m3)
- GGBFS (kg/m3)
- Coarse aggregate (kg/m3)

2 - Specify target values

Show / hide dataset for editing

Formulation Index	Feature Summary	X
0	Idx_Sample: 1399.0, SiO2: 52.295, CaO: 12.58, SO3: 0.27, FA (kg/m3): 252.0, GGBFS (kg/m3): 108.0, Coarse aggregate (kg/m3): 1090.8, Fine aggregate (kg/m3): 774.0, Total aggregates: 1864.8, Na2SiO3: 115.71429, Na2O (Dry): 13.31, Sio2 (Dry): 34.71, Superplasticizer: 14.4, water -eff: 107.80714, Slump - Target (mm): nan, CO2 (kg/t) - A-priori Information: 112.66807, fc 28-d - Target (MPa): nan, X: nan	<div></div>
1	Idx_Sample: 1400.0, SiO2: 52.295, CaO: 12.58, SO3: 0.27, FA (kg/m3): 252.0, GGBFS (kg/m3): 108.0, Coarse aggregate (kg/m3): 1090.8, Fine aggregate (kg/m3): 774.0, Total aggregates: 1864.8, Na2SiO3: 128.57143, Na2O (Dry): 14.79, Sio2 (Dry): 38.57, Superplasticizer: 14.4, water -eff: 118.82571, Slump - Target (mm): nan, CO2 (kg/t) - A-priori Information: 120.44818, fc 28-d - Target (MPa): nan, X: nan	<div></div>

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 pre-filled. 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.

6.2 Configuring and running 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 below 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.

Show / hide materials discovery explanation

Materials Data (Input) (select one column at least)

Fine aggregate (kg/m3)
Total aggregates
Na2SiO3
Na2O (Dry)
Sio2 (Dry)
Superplasticizer
water -eff

Target Properties (select one column at least)

Idx_Sample
Slump - Target (mm)
CO2 (kg/t) - A-priori Information
fc 28-d - Target (MPa)
X

A priori Information (optional)

Idx_Sample
CO2 (kg/t) - A-priori Information
X

Slump - Target (mm)

☒ Maximize

☐ Minimize

Weight

1.00

Threshold

Optional

fc 28-d - Target (MPa)

☒ Maximize

☐ Minimize

Weight

1.5

Threshold

Optional

CO2 (kg/t) - A-priori Information

☐ Maximize

☒ Minimize

Weight

1.00

Threshold

Optional

Select Model *

Statistics-based model (Gaussian Process Regression)

Curiosity (to control the weight of model uncertainty on predicted utility) *

Exploit 1.0 Explore

Run experiment with given configuration

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.

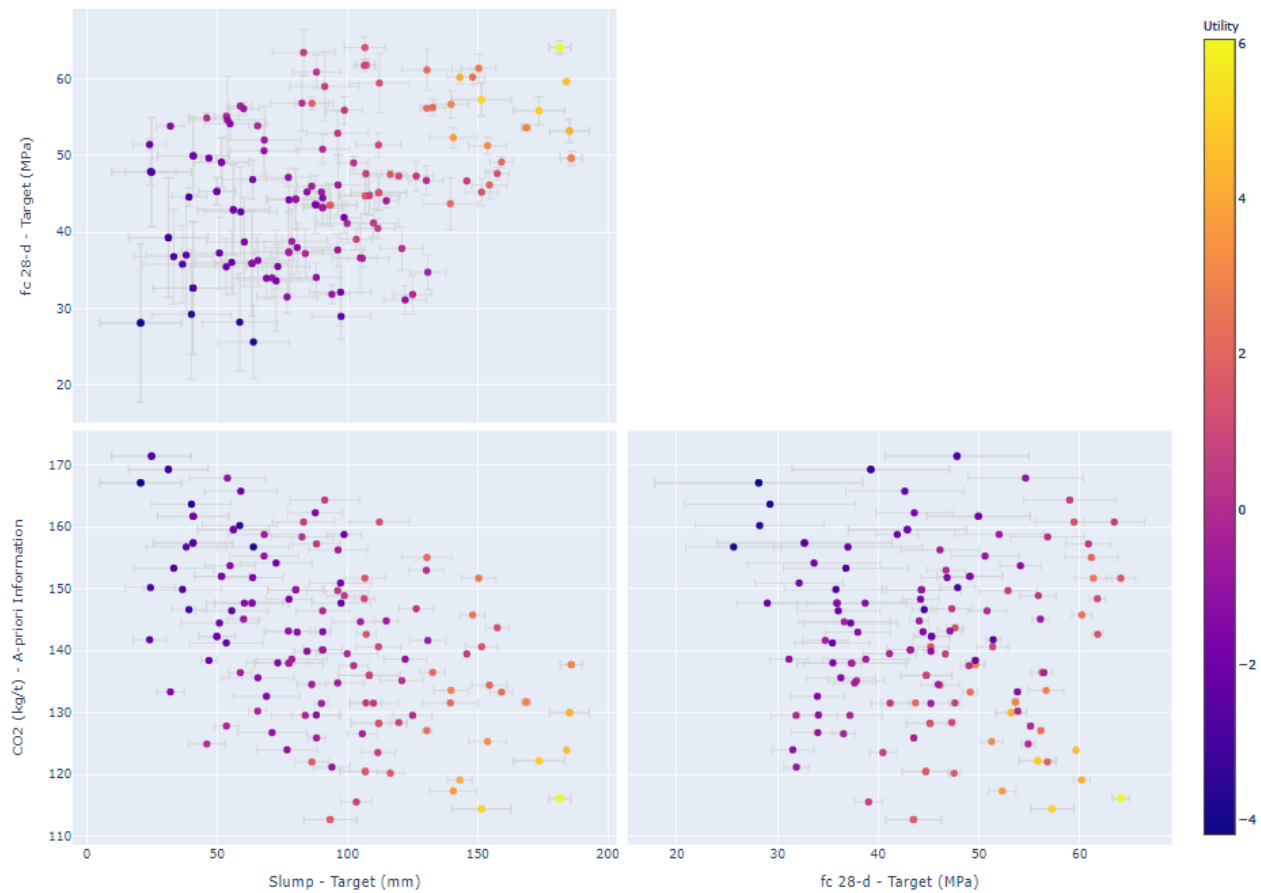
Row number	Utility	Novelty	Slump - Target (mm)	fc 28-d - Target (MPa)	Uncertainty (Slump - Target (mm))	Uncertainty (fc 28-d - Target (MPa))	Idx_Sample	SiO2	CaO	SO3	FA (kg/m3)	GGBFS (kg/m3)	Coarse aggregate (kg/m3)	Fine aggregate (kg/m3)	agg
1	2.946420	0.523664	112.342442	59.452994	23.26243	7.68811	1430	47.085	18.30	0.45	210	210	966.00000	810.60000	1776
2	2.808785	0.620889	91.353715	59.014729	26.62892	9.16342	1588	47.085	18.30	0.45	215	215	967.96105	795.03895	1763
3	2.722163	0.262025	150.456857	61.376902	13.29414	3.70176	1429	47.085	18.30	0.45	210	210	966.00000	810.60000	1776
4	2.709731	0.401033	130.591258	61.171319	19.37737	5.30052	1558	47.085	18.30	0.45	215	215	967.96105	795.03895	1763

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.

Download Predictions

Utility in output space (Scatter matrix / plot)

Scatter matrix of target properties



Utility in input space (t-SNE plot)