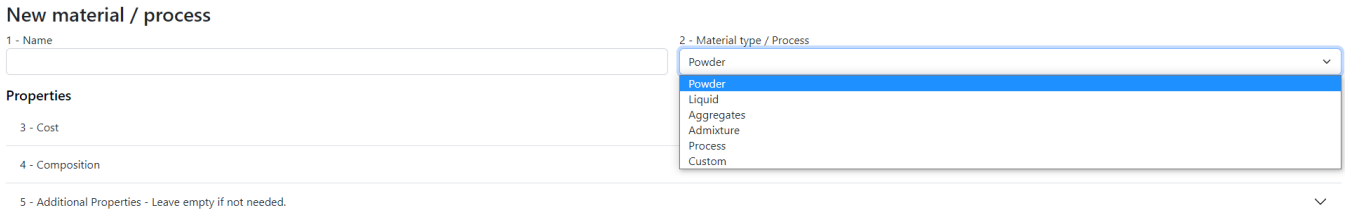
User Manual

Based on the functionality provided with SLAMD, this document provides a guide of how to use the app.

The general workflow is as follows. First define base materials and processes. Then, you use the former as a basis to create blended materials. Next, a materials
formulations can be specified. For this purpose one selects a subset of all materials and processes created. The resulting data can but must not be enriched with targets (labels).
This specification of data can now used in the sequential learning for the prediction of new material properties.

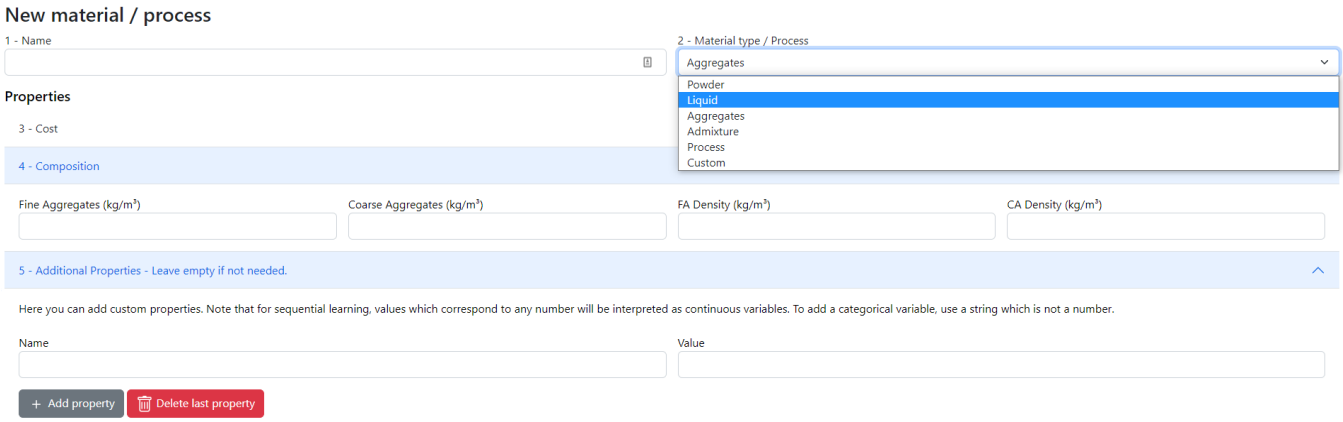
Base Materials and Processes

The starting point is the creation of base materials and processes. Here you can first select the type of base material or process you want to specify.



Note that for all the types you can specify a name, costs and additional properties in the same way. The concrete composition, however, depends on the type (e.g. in the screenshow below, aggregates is shown.
Furthermore, there is the possibility to specify custom materials. These are not restricted and can in principle describe any type of material. As such, it has no a priori composition and must thus be specified in terms
of its additional properties solely. Note that the latter can be used to specify a custom composition anyway.

You can open the cost / composition / additional properties input fields by clicking on the corresponding item below "Properties".



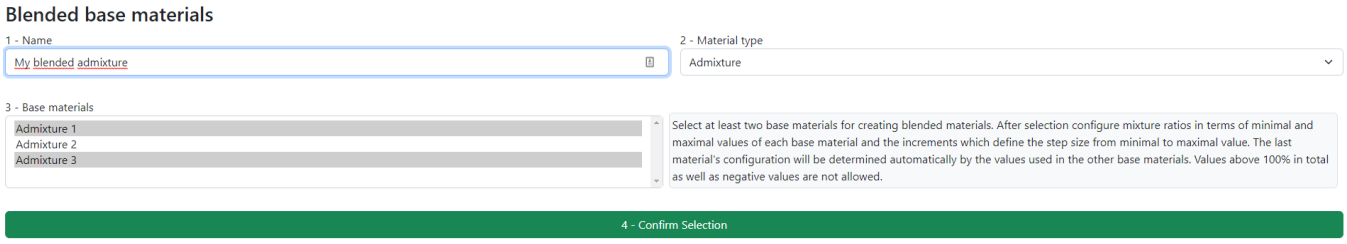
Depending on the field, either only numerical or any alphanumeric input can be specified. Note that for later creation of blended materials, a base materials with
at least one field empty (in costs or composition) is considered incomplete and a warning is shown. Nevertheless blending can be still be performed as one might not want to create base materials
and blends consisting of all the possible features. More details on blending rules will be specified below.

The additional properties (at most 10!) allow defining additonal custom features for the material. In principle, you are free to specify any name and corrsponding value. Note however, that when blending
there are again certain rules which apply. For a complete description the names and corresponding value types must match across all base materials used for blending.

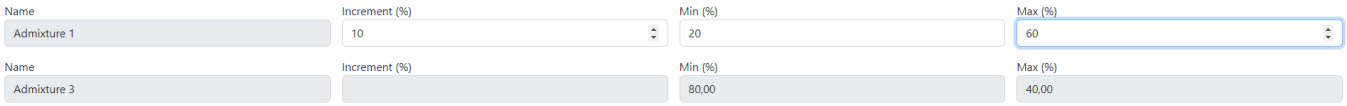
Having configured your material you can save it by clicking on the "Save material" button. The new item appears in the table showing all base materials and processes. In the left column you have functionalities
to delete or edit the chosen material. In case of clicking the edit button, the form will be populated by the previously configured data.

Blended Materials

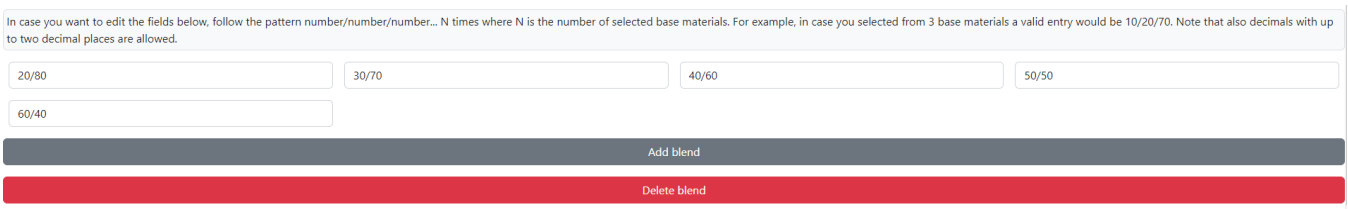
The next step is creating blended materials. As a starting point set a name (mandatory) and a type and choose at least two base materials:



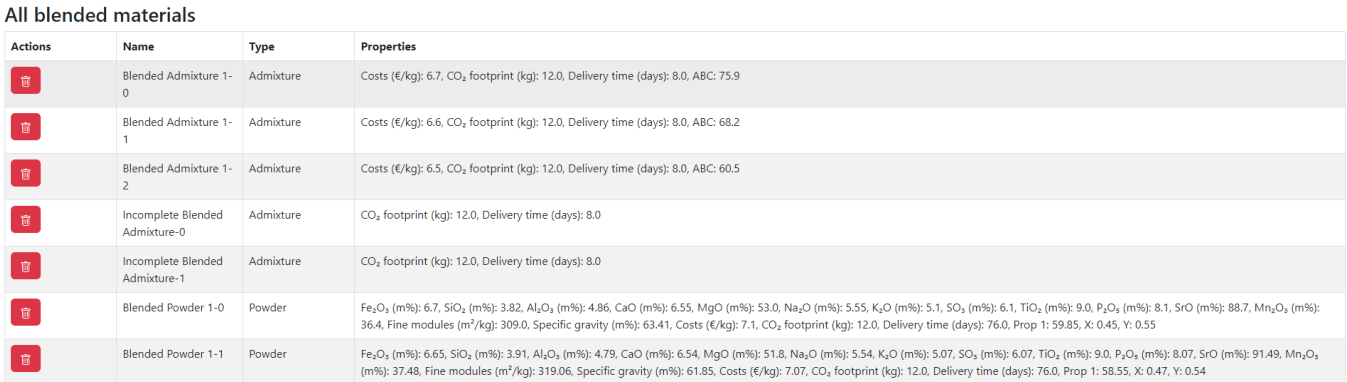
Blending then basically corresponds to mixing different materials of a given type with one another to create materials with various ratios of the properties for all base materials involved.
For example, in case of the hypothetical situation where you have two powders both solely described by 'Specific 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. Note that 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.



The relative ratios can be specified after having selected the base materials used for blending. Note that the last row is always determined by the previous ones. In the screenshot, e.g. we blend from two base admixtures (in general, we can use more than just two).
The min and max values of the last material are determined by the constrained that the sum over all has to equal 100%. Accordingly, one can only specify values and increments for the independent materials. The resulting ratios are computed as the direct product of all possibilities, e.g. in the scenario shown in the above image we get



If we were to submit this configuration, we would generate five blended admixtures. Note, however, that it is still possible to add, delete and edit the mixtures. Here, there is no more restriction that everything needs to add up to 100. However, one must follow the correct pattern when editing (as shown in the comment in the screenshot).
Finally, once you are finished with the specification of the blending configuration, click the "Create blended materials" button to create your blends. The created entries are saved and displayed in a table which show all details (here we show some blended materials which we have already created):



In addition, there are several rules which apply when not all fields are filled in the base materials or in case some properties are only filled for one of the base materials to be mixed.

- A description is complete only when all input fields are filled (except for additional properties)
- Assume you want to mix two (or more) base materials which both define a compositional / costs or structural property which we call 'Base Material Property' in the following (it could e.g. be Specific Gravity in case of powders)
  and assume both define an additional property calles 'Add. Prop'. Then the following rules apply when blending:

  a) 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
  b) 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
  c) Add. Prop is filled for all base materials and has only numeric value the resulting blended materials have the property Add. Prop computed as the weighted sum of its base materials Add. Prop values
  d) Add. Prop is filled for all base materials and has only non-numeric values a new Property for all differing values of the corresponding base

materials Add. Prop will be created with the value set by the relative weight of the base material. E.g if we have two powders,
Powder A and Powder B and Add. Prop of Powder A is set as X and Add. Prop of Powder B is set as Y and we have a mixing ratio of 20/80 then the resulting blend does not have an additional property Add. Prop but rather two additional properties X and Y with values 0.2
and 0.8, respectively. This is also illustrated in the images below for the additional property 'Prop 2' (here, we have two base materials and the weights configured such that three blended materials are created from these).
e) 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

	Powder 1	Powder	Fe_2O_3 (m%): 5.1, SiO_2 (m%): 7.0, Al_2O_3 (m%): 2.1, CaO (m%): 6.0, MgO (m%): 9.0, Na_2O (m%): 5.0, K_2O (m%): 4.0, SO_3 (m%): 5.0, TiO_2 (m%): 9.0, P_2O_5 (m%): 7.0, SrO (m%): 191.0, Mn_2O_3 (m%): 76.0, Fine modules (m^2/kg): 678.1, Specific gravity (m%): 6.22, Costs (€/kg): 6.0, CO_2 footprint (kg): 12.0, Delivery time (days): 76.0, Prop 1: 12, Prop 2: X
	Powder 2	Powder	Fe_2O_3 (m%): 8.0, SiO_2 (m%): 1.22, Al_2O_3 (m%): 7.12, CaO (m%): 7.0, MgO (m%): 89.0, Na_2O (m%): 6.0, K_2O (m%): 6.0, SO_3 (m%): 7.0, TiO_2 (m%): 9.0, P_2O_5 (m%): 9.0, SrO (m%): 5.0, Mn_2O_3 (m%): 4.0, Fine modules (m^2/kg): 7.0, Specific gravity (m%): 110.2, Costs (€/kg): 8.0, CO_2 footprint (kg): 12.0, Delivery time (days): 1.0, Prop 1: 99, Prop 2: Y

	Blended Powder 1-0	Powder	Fe_2O_3 (m%): 6.7, SiO_2 (m%): 3.82, Al_2O_3 (m%): 4.86, CaO (m%): 6.55, MgO (m%): 53.0, Na_2O (m%): 5.55, K_2O (m%): 5.1, SO_3 (m%): 6.1, TiO_2 (m%): 9.0, P_2O_5 (m%): 8.1, SrO (m%): 88.7, Mn_2O_3 (m%): 36.4, Fine modules (m^2/kg): 309.0, Specific gravity (m%): 63.41, Costs (€/kg): 7.1, CO_2 footprint (kg): 12.0, Delivery time (days): 76.0, Prop 1: 59.85, X: 0.45, Y: 0.55
	Blended Powder 1-1	Powder	Fe_2O_3 (m%): 6.65, SiO_2 (m%): 3.91, Al_2O_3 (m%): 4.79, CaO (m%): 6.54, MgO (m%): 51.8, Na_2O (m%): 5.54, K_2O (m%): 5.07, SO_3 (m%): 6.07, TiO_2 (m%): 9.0, P_2O_5 (m%): 8.07, SrO (m%): 91.49, Mn_2O_3 (m%): 37.48, Fine modules (m^2/kg): 319.06, Specific gravity (m%): 61.85, Costs (€/kg): 7.07, CO_2 footprint (kg): 12.0, Delivery time (days): 76.0, Prop 1: 58.55, X: 0.47, Y: 0.54
	Blended Powder 1-2	Powder	Fe_2O_3 (m%): 6.61, SiO_2 (m%): 3.99, Al_2O_3 (m%): 4.71, CaO (m%): 6.52, MgO (m%): 50.6, Na_2O (m%): 5.52, K_2O (m%): 5.04, SO_3 (m%): 6.04, TiO_2 (m%): 9.0, P_2O_5 (m%): 8.04, SrO (m%): 94.28, Mn_2O_3 (m%): 38.56, Fine modules (m^2/kg): 329.13, Specific gravity (m%): 60.29, Costs (€/kg): 7.04, CO_2 footprint (kg): 12.0, Delivery time (days): 76.0, Prop 1: 57.24, X: 0.48, Y: 0.52
	Blended Powder 1-3	Powder	Fe_2O_3 (m%): 6.56, SiO_2 (m%): 4.08, Al_2O_3 (m%): 4.64, CaO (m%): 6.5, MgO (m%): 49.4, Na_2O (m%): 5.51, K_2O (m%): 5.01, SO_3 (m%): 6.01, TiO_2 (m%): 9.0, P_2O_5 (m%): 8.01, SrO (m%): 97.07, Mn_2O_3 (m%): 39.64, Fine modules (m^2/kg): 339.19, Specific gravity (m%): 58.73, Costs (€/kg): 7.01, CO_2 footprint (kg): 12.0, Delivery time (days): 76.0, Prop 1: 55.93, X: 0.49, Y: 0.51

Note that whenever a configuration of base materials is chosen leading any of the described incomplete scenarios, a warning is shown.

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.

Name	Increment (%)	Min (%)	Max (%)
Admixture 1			

Name	Increment (%)	Min (%)	Max (%)
Admixture 3			