26.01.2023

DATA DRIVEN MATERIALS DESIGN PART III.

Dr. Christoph Völker

christoph.voelker@bam.de

Ressources

Materials Design App

SLAMD: https://slamd-demo.herokuapp.com/

Data: https://github.com/BAMcvoelker/Praktikum_MD/

- *SessionExample.json* <- a SLAMD session file that contains some of the materials
- *SessionComplete.json* <- a SLAMD session file that contains the complete list of materials and materials blends that are required to create the geopolymer based concrete formulation
- *DiscoveryData_Sample.csv* <- a materials data search space with labels
- Slides

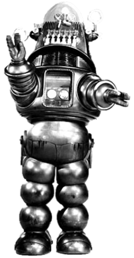
Scope

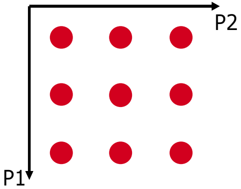
I. Part (Lecture) Introduction to data driven materials design

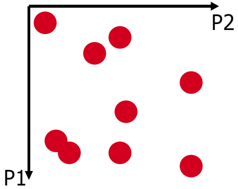
II. Part (Lecture) Advanced methods

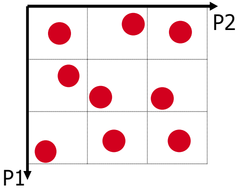
III. Hands on

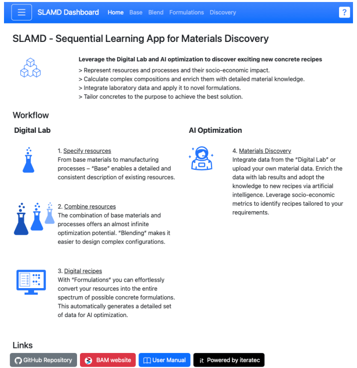
- AI-driven materials design with SLAMD
- How to?
- Practical example











SLAMD - Sequential Learning App for Materials Discovery

Leverage the Digital Lab and AI optimization to discover exciting new concrete recipes

> Represent resources and processes and their socio-economic impact.
> Calculate complex compositions and enrich them with detailed material knowledge.
> Integrate laboratory data and apply it to novel formulations.
> Tailor concretes to the purpose to achieve the best solution.

Workflow

Digital Lab

1. Specify resources
From base materials to manufacturing processes – "Base" enables a detailed and consistent description of existing resources.

2. Combine resources
The combination of base materials and processes offers an almost infinite optimization potential. "Blending" makes it easier to design complex configurations.

3. Digital recipes
With "Formulations" you can effortlessly convert your resources into the entire spectrum of possible concrete formulations. This automatically generates a detailed set of data for AI optimization.

AI Optimization

4. Materials Discovery
Integrate data from the "Digital Lab" or upload your own material data. Enrich the data with lab results and adopt the knowledge to new recipes via artificial intelligence. Leverage socio-economic metrics to identify recipes tailored to your requirements.

Links

SLAMD Workflow

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Links

Link:
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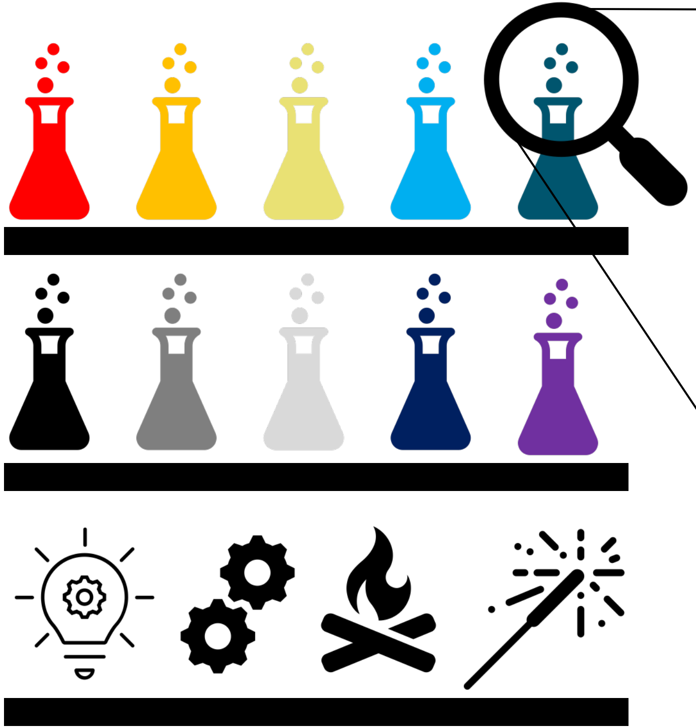
Digital Lab



Digital Twin

👩‍🔬 **Materials prop.**

🧪 ………% CaO

……… $\% \, SiO_2$

🔍 ……… $^{mm^2}/_{g}$

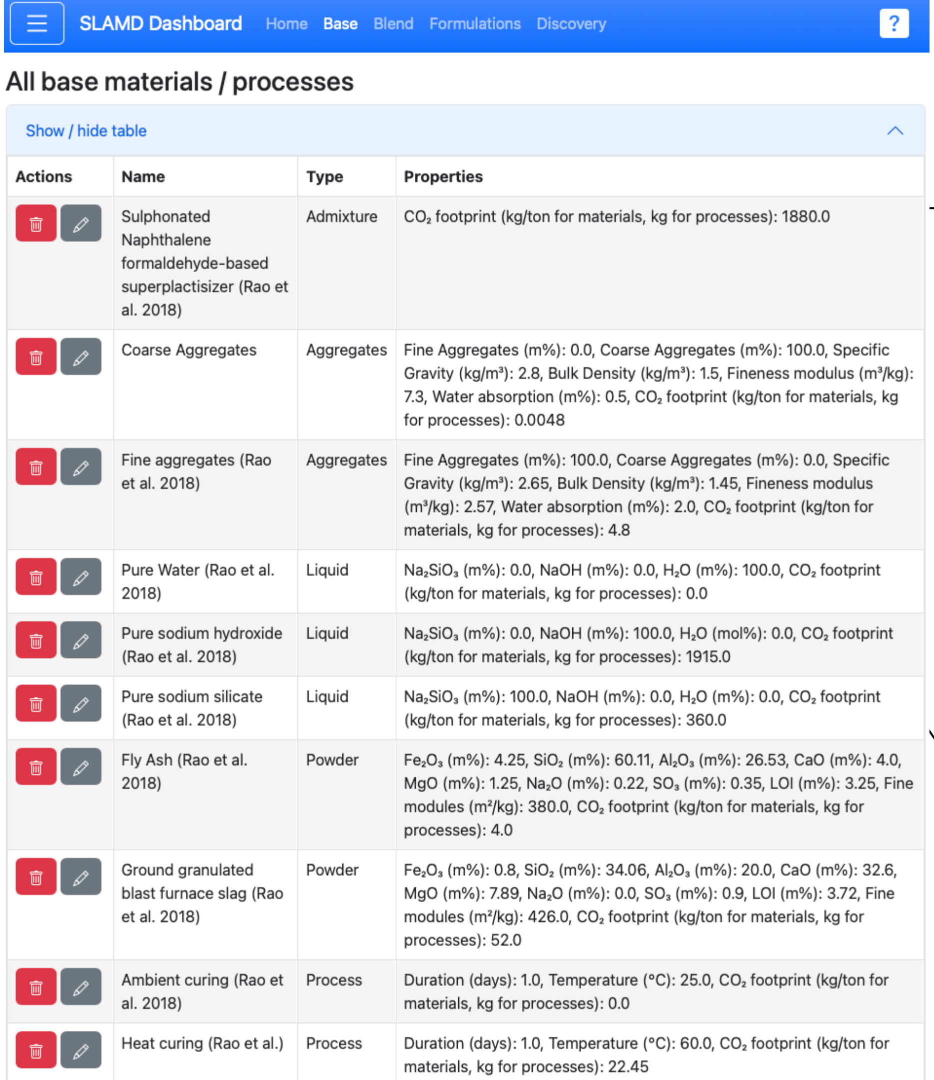
🎨 ………

👨‍💻 **Socio-eco. prop.**

🍀 ……… $kgCO_2$

💰 ……… €

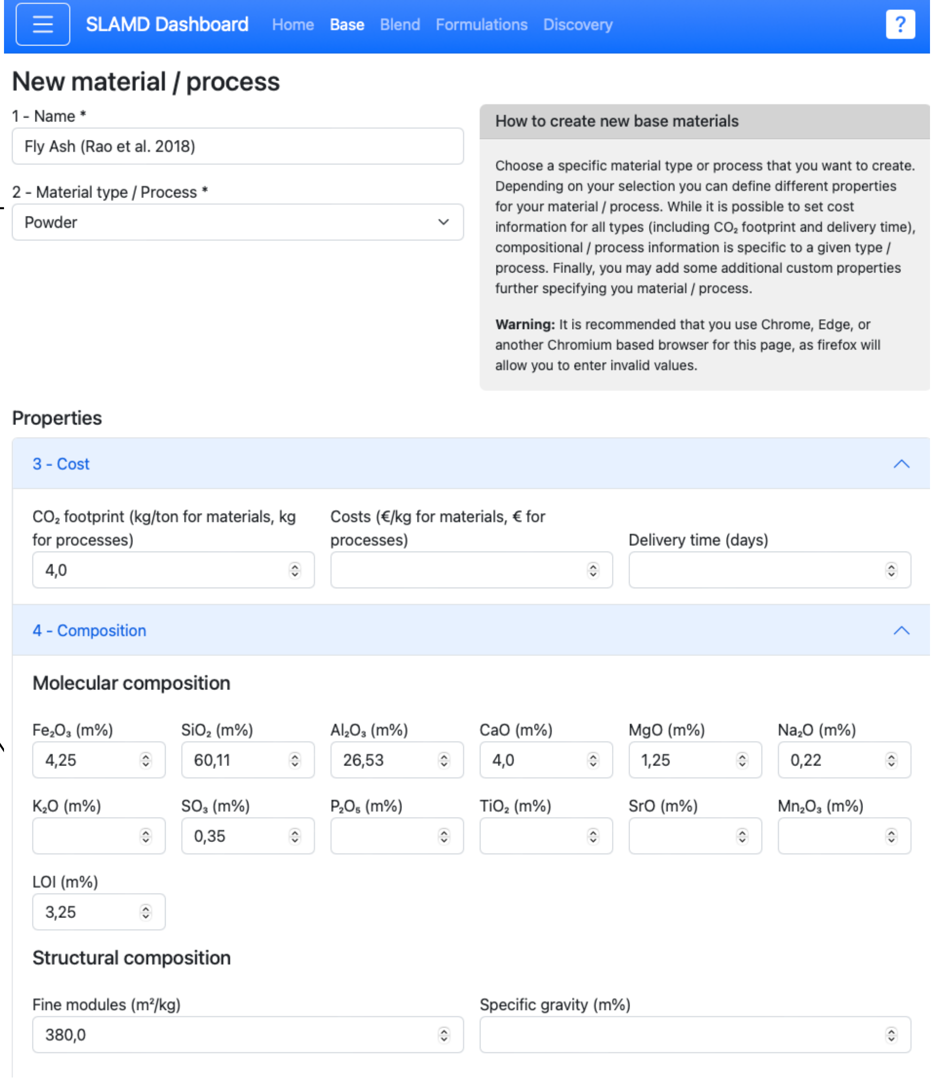
♻️ ……… %



All base materials / processes

Show / hide table

Actions	Name	Type	Properties
	Sulphonated Naphthalene formaldehyde-based superplactisizer (Rao et al. 2018)	Admixture	CO_2 footprint (kg/ton for materials, kg for processes): 1880.0
	Coarse Aggregates	Aggregates	Fine Aggregates (m%): 0.0, Coarse Aggregates (m%): 100.0, Specific Gravity (kg/m³): 2.8, Bulk Density (kg/m³): 1.5, Fineness modulus (m³/kg): 7.3, Water absorption (m%): 0.5, CO_2 footprint (kg/ton for materials, kg for processes): 0.0048
	Fine aggregates (Rao et al. 2018)	Aggregates	Fine Aggregates (m%): 100.0, Coarse Aggregates (m%): 0.0, Specific Gravity (kg/m³): 2.65, Bulk Density (kg/m³): 1.45, Fineness modulus (m³/kg): 2.57, Water absorption (m%): 2.0, CO_2 footprint (kg/ton for materials, kg for processes): 4.8
	Pure Water (Rao et al. 2018)	Liquid	Na_2SiO_3 (m%): 0.0, NaOH (m%): 0.0, H_2O (m%): 100.0, CO_2 footprint (kg/ton for materials, kg for processes): 0.0
	Pure sodium hydroxide (Rao et al. 2018)	Liquid	Na_2SiO_3 (m%): 0.0, NaOH (m%): 100.0, H_2O (mol%): 0.0, CO_2 footprint (kg/ton for materials, kg for processes): 1915.0
	Pure sodium silicate (Rao et al. 2018)	Liquid	Na_2SiO_3 (m%): 100.0, NaOH (m%): 0.0, H_2O (m%): 0.0, CO_2 footprint (kg/ton for materials, kg for processes): 360.0
	Fly Ash (Rao et al. 2018)	Powder	Fe_2O_3 (m%): 4.25, SiO_2 (m%): 60.11, Al_2O_3 (m%): 26.53, CaO (m%): 4.0, MgO (m%): 1.25, Na_2O (m%): 0.22, SO_3 (m%): 0.35, LOI (m%): 3.25, Fine modules (m²/kg): 380.0, CO_2 footprint (kg/ton for materials, kg for processes): 4.0
	Ground granulated blast furnace slag (Rao et al. 2018)	Powder	Fe_2O_3 (m%): 0.8, SiO_2 (m%): 34.06, Al_2O_3 (m%): 20.0, CaO (m%): 32.6, MgO (m%): 7.89, Na_2O (m%): 0.0, SO_3 (m%): 0.9, LOI (m%): 3.72, Fine modules (m²/kg): 426.0, CO_2 footprint (kg/ton for materials, kg for processes): 52.0
	Ambient curing (Rao et al. 2018)	Process	Duration (days): 1.0, Temperature (°C): 25.0, CO_2 footprint (kg/ton for materials, kg for processes): 0.0
	Heat curing (Rao et al.)	Process	Duration (days): 1.0, Temperature (°C): 60.0, CO_2 footprint (kg/ton for materials, kg for processes): 22.45



New material / process

1 - Name *: Fly Ash (Rao et al. 2018)

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 CO_2 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

CO_2 footprint (kg/ton for materials, kg for processes): 4,0
Costs (€/kg for materials, € for processes):
Delivery time (days):

4 - Composition

Molecular composition

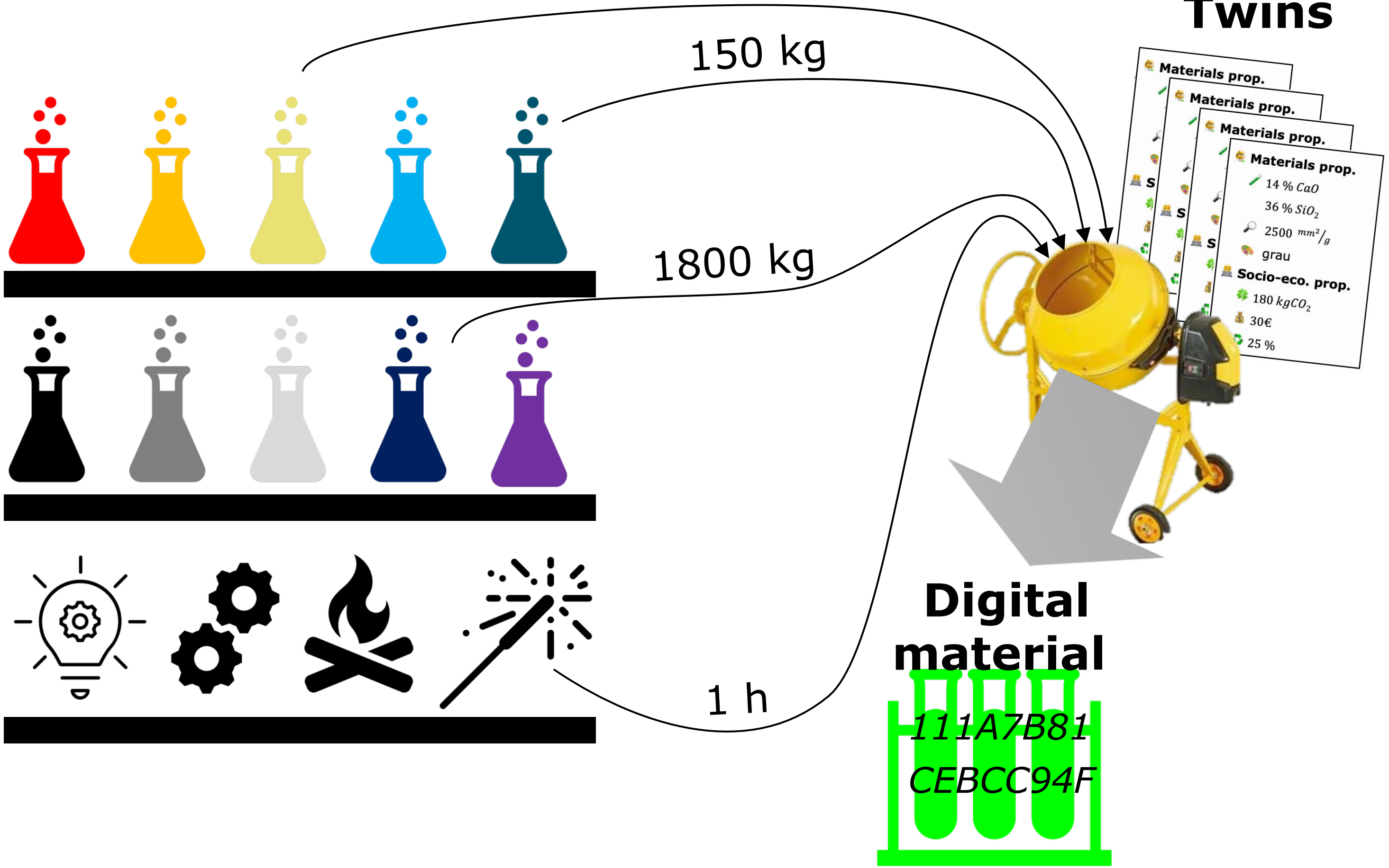
Fe_2O_3 (m%): 4,25
SiO_2 (m%): 60,11
Al_2O_3 (m%): 26,53
CaO (m%): 4,0
MgO (m%): 1,25
Na_2O (m%): 0,22
K_2O (m%):
SO_3 (m%): 0,35
P_2O_5 (m%):
TiO_2 (m%):
SrO (m%):
Mn_2O_3 (m%):
LOI (m%): 3,25

Structural composition

Fine modules (m²/kg): 380,0
Specific gravity (m%):

Digital Lab

Digital Twins



Materials prop.
- 14 % CaO
- 36 % SiO_2
- 2500 $^{mm^2}/_g$
- grau

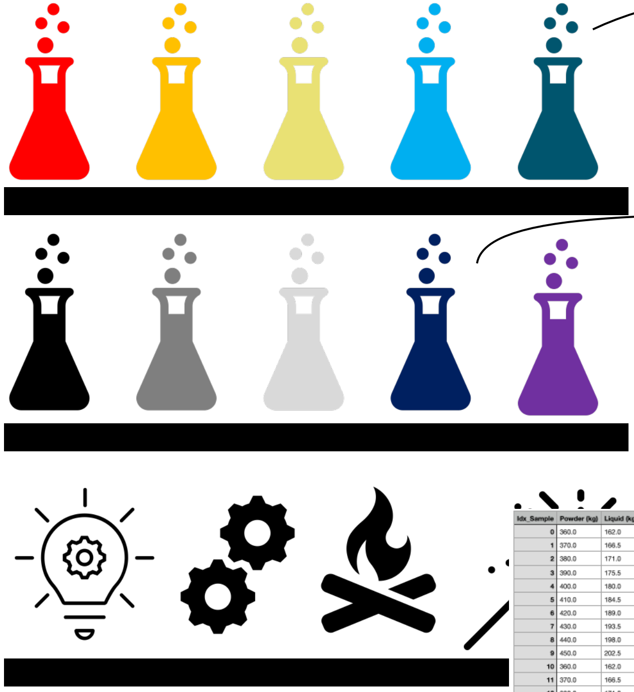
Socio-eco. prop.
- 180 $kgCO_2$
- 30€
- 25 %

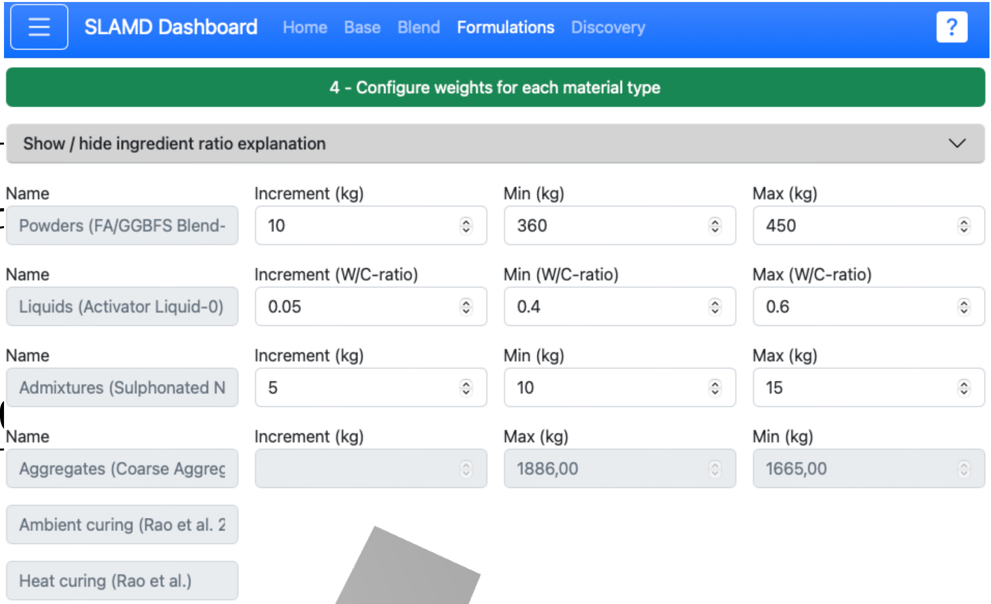
Digital Lab

300

1

18





Name: Powders (FA/GGBFS Blend-
Increment (kg): 10
Min (kg): 360
Max (kg): 450

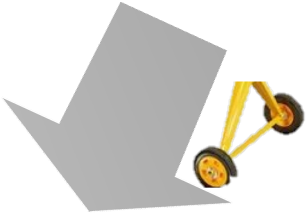
Name: Liquids (Activator Liquid-0)
Increment (W/C-ratio): 0.05
Min (W/C-ratio): 0.4
Max (W/C-ratio): 0.6

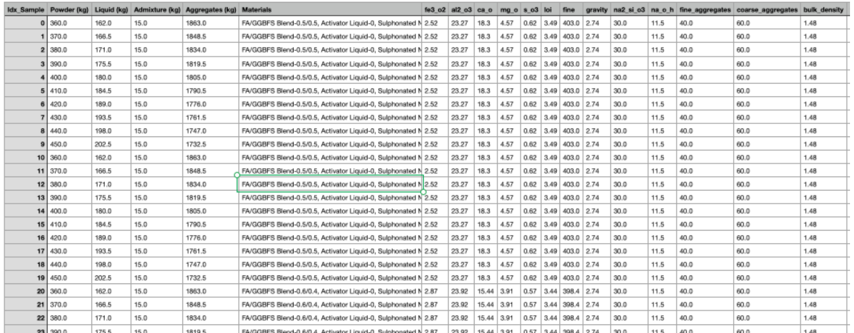
Name: Admixtures (Sulphonated N
Increment (kg): 5
Min (kg): 10
Max (kg): 15

Name: Aggregates (Coarse Aggreg
Increment (kg):
Max (kg): 1886,00
Min (kg): 1665,00

Ambient curing (Rao et al. 2

Heat curing (Rao et al.)





Idx_Sample	Powder (kg)	Liquid (kg)	Admixture (kg)	Aggregates (kg)	Materials	fe3_o2	al2_o3	ca_o	mg_o	s_o3	loi	fine	gravity	na2_si_o3	na_o_h	fine_aggregates	coarse_aggregates	bulk_density
0	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
1	370.0	166.5	15.0	1848.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
2	380.0	171.0	15.0	1834.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
3	390.0	175.5	15.0	1819.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
4	400.0	180.0	15.0	1805.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
5	410.0	184.5	15.0	1790.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
6	420.0	189.0	15.0	1776.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
7	430.0	193.5	15.0	1761.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
8	440.0	198.0	15.0	1747.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
9	450.0	202.5	15.0	1732.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
10	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
11	370.0	166.5	15.0	1848.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
12	380.0	171.0	15.0	1834.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
13	390.0	175.5	15.0	1819.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
14	400.0	180.0	15.0	1805.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
15	410.0	184.5	15.0	1790.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
16	420.0	189.0	15.0	1776.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
17	430.0	193.5	15.0	1761.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
18	440.0	198.0	15.0	1747.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
19	450.0	202.5	15.0	1732.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
20	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48
21	370.0	166.5	15.0	1848.5	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48
22	380.0	171.0	15.0	1834.0	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48
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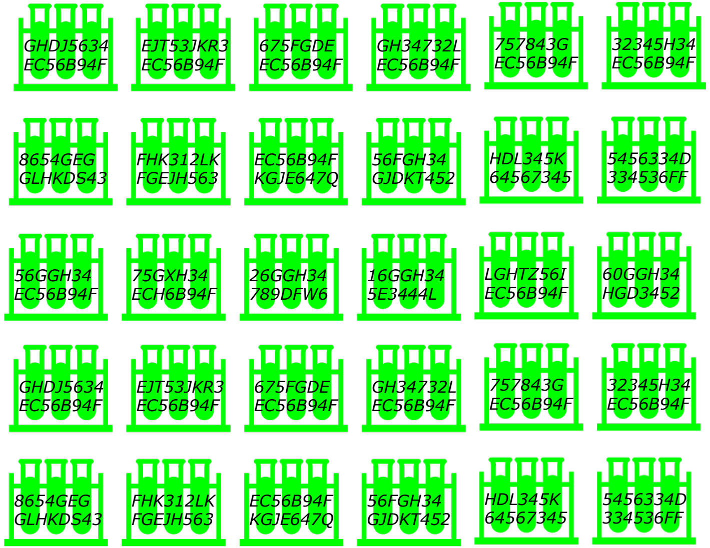
AI Optimization - Materials discovery dashboard

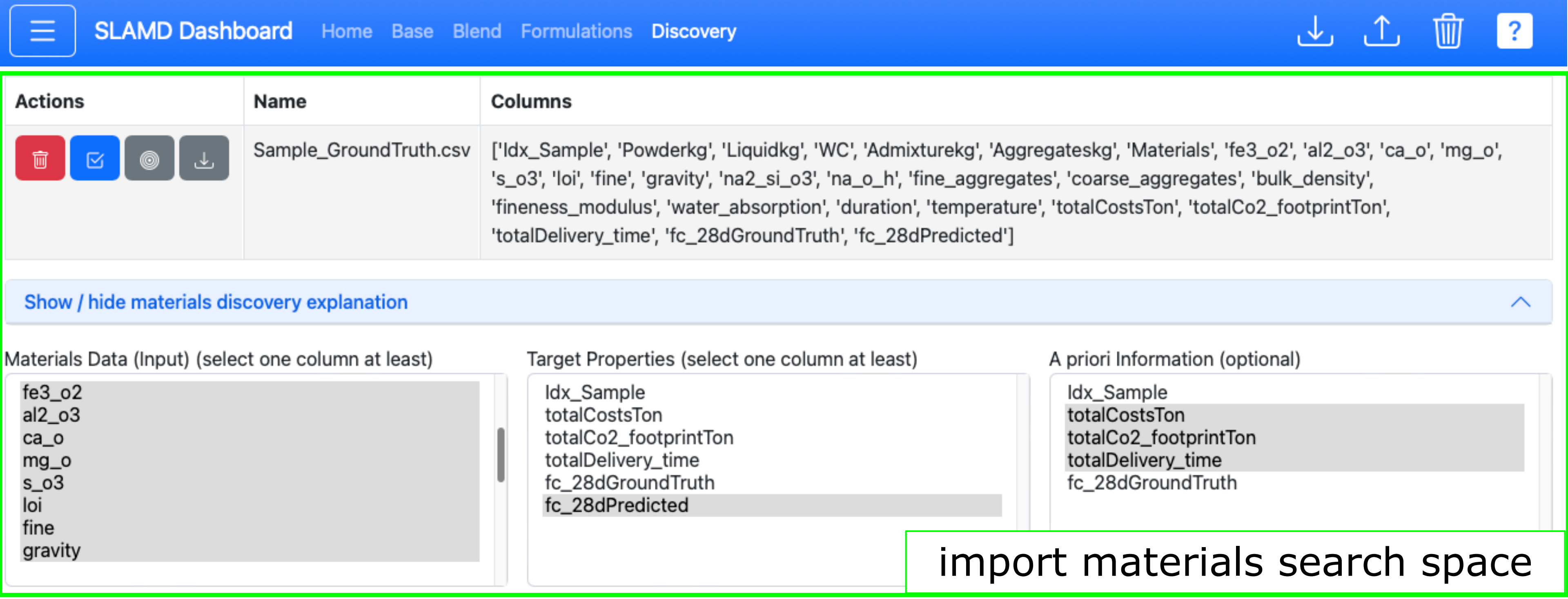
Import materials search space



Set objectives

Strenght (Maximize)
Threshold: 45 MPa

Costs (Minimize)
Threshold: 90 €
CO2-Footprint (Minimize)
Threshold: 120 kg/ton



Actions	Name	Columns
	Sample_GroundTruth.csv	['Idx_Sample', 'Powderkg', 'Liquidkg', 'WC', 'Admixturekg', 'Aggregateskg', 'Materials', 'fe3_o2', 'al2_o3', 'ca_o', 'mg_o', 's_o3', 'loi', 'fine', 'gravity', 'na2_si_o3', 'na_o_h', 'fine_aggregates', 'coarse_aggregates', 'bulk_density', 'fineness_modulus', 'water_absorption', 'duration', 'temperature', 'totalCostsTon', 'totalCo2_footprintTon', 'totalDelivery_time', 'fc_28dGroundTruth', 'fc_28dPredicted']

Show / hide materials discovery explanation

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

- fe3_o2
- al2_o3
- ca_o
- mg_o
- s_o3
- loi
- fine
- gravity

Target Properties (select one column at least)

- Idx_Sample
- totalCostsTon
- totalCo2_footprintTon
- totalDelivery_time
- fc_28dGroundTruth
- fc_28dPredicted

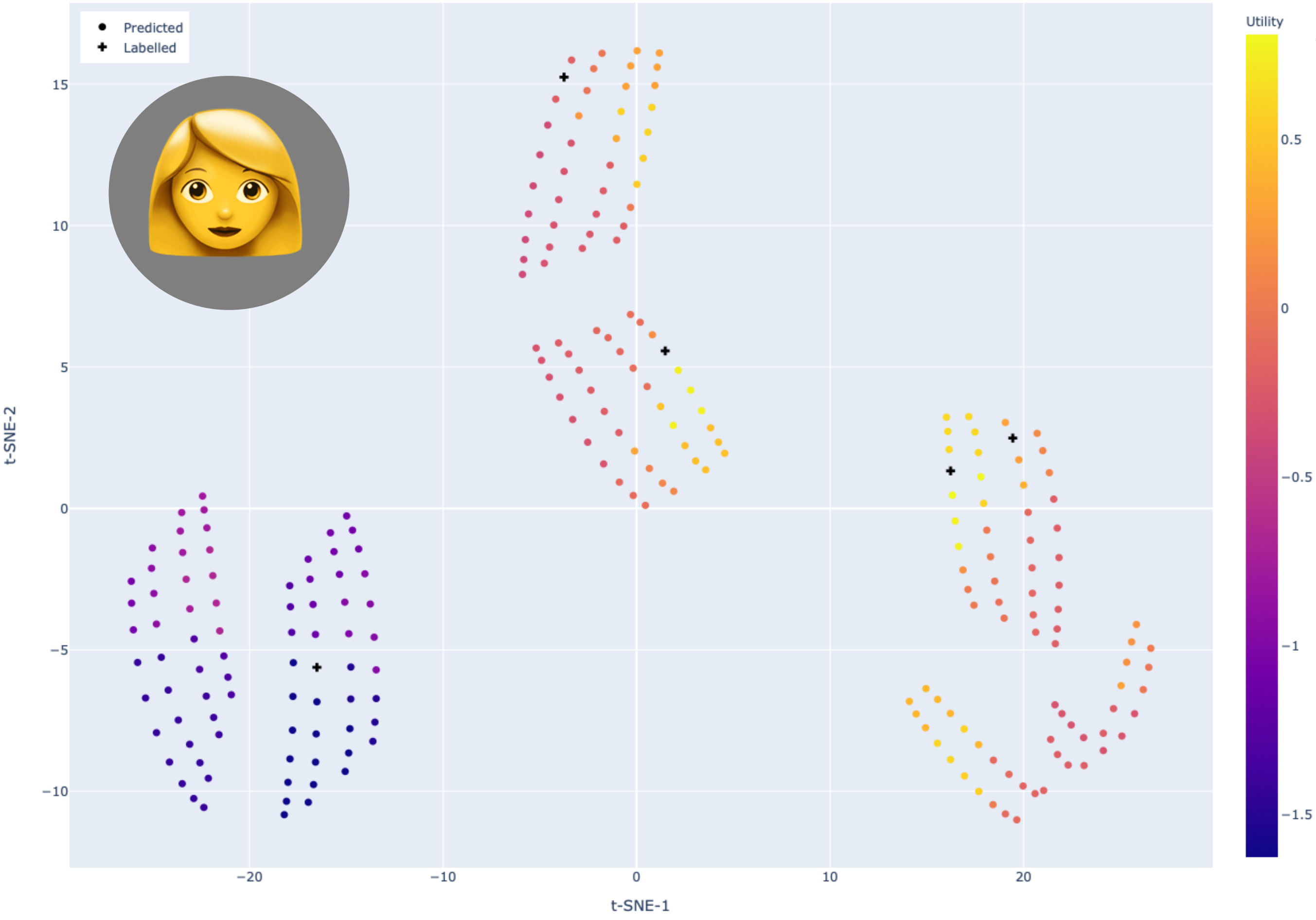
A priori Information (optional)

- Idx_Sample
- totalCostsTon
- totalCo2_footprintTon
- totalDelivery_time
- fc_28dGroundTruth

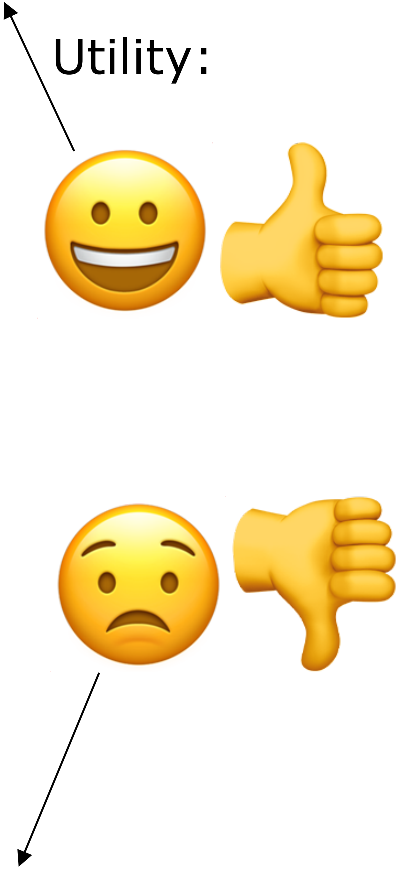
import materials search space

fc_28dPredicted	● Maximize	○ Minimize	Weight 1,00	Threshold 45
totalCostsTon	○ Maximize	● Minimize	Weight 1,00	Threshold 90
totalCo2_footprintTon	○ Maximize	● Minimize	Weight 1,00	Threshold 120
totalDelivery_time	○ Maximize	● Minimize	Weight 1,00	Threshold 5

Material search space



Utility:



How to

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How to?

The configuration of the optimization problem is the key to its success. Here is some advice base on a large scale literature study where we have probed questions such as:

Q1: Which **ML-algorithm**?

Q2: How much **training data**?

Q3: Does **informed AI** improve performance?

9

search spaces*

1… 10 …20

ref’s from literature

90 … 152 … 274

recipes

28 … 37 … 43

parameters

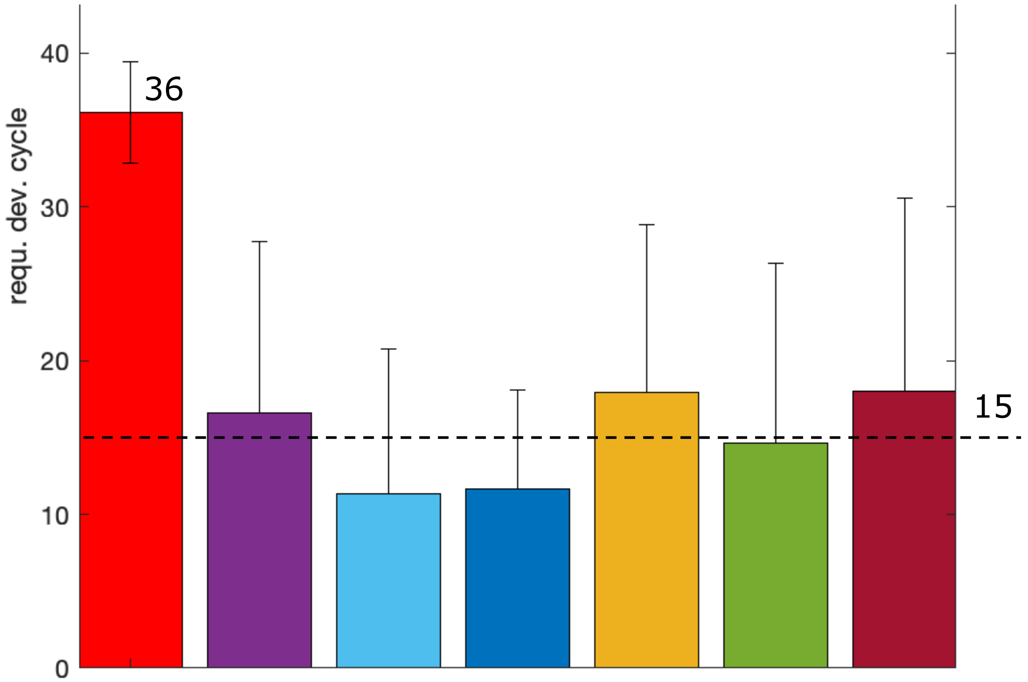
compressive strength (MPa)

CO_2 footprint (kg/ton)

Benchmarking (required development cycle)

*https://github.com/BAMcvoelker/SLAMD-FIB-Case-Study

Q1: Algorithm



Mean required development cycle to reach top 5% performance with 90% certainty.

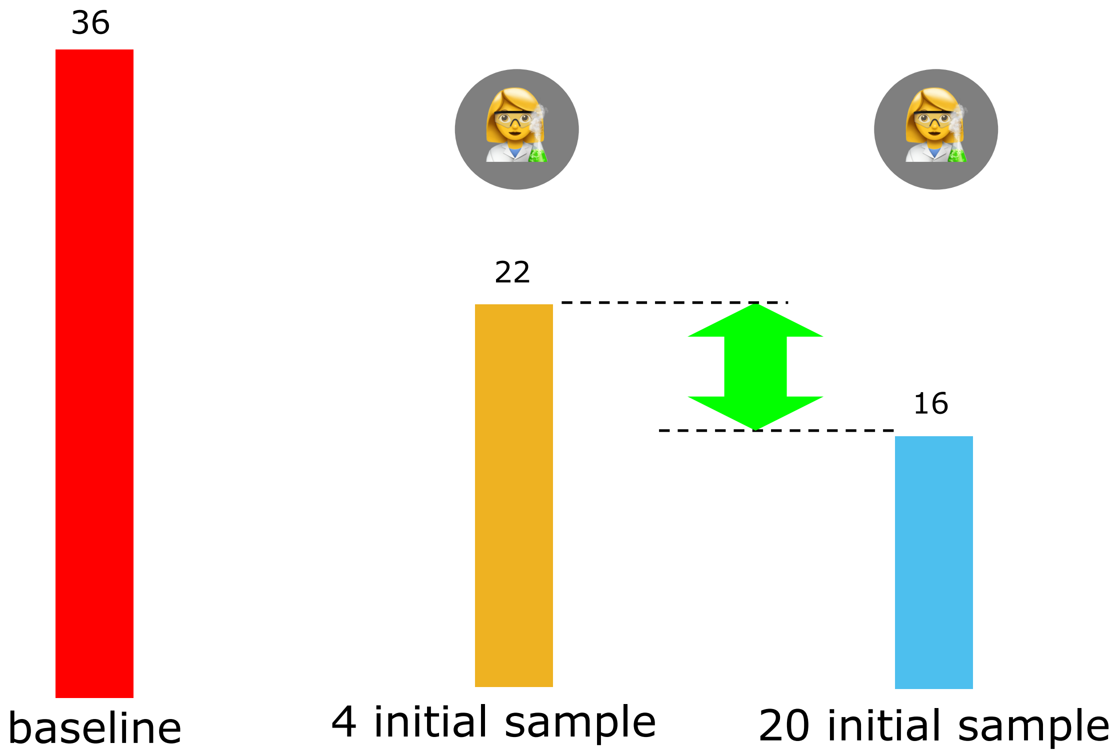
$$9\ data\ sets\ *$$

$$4\ scenarios\ *$$

$$25\ randomized\ runs\ =$$

$$\underline{\mathbf{900}\ Experiments/Algorithm}$$

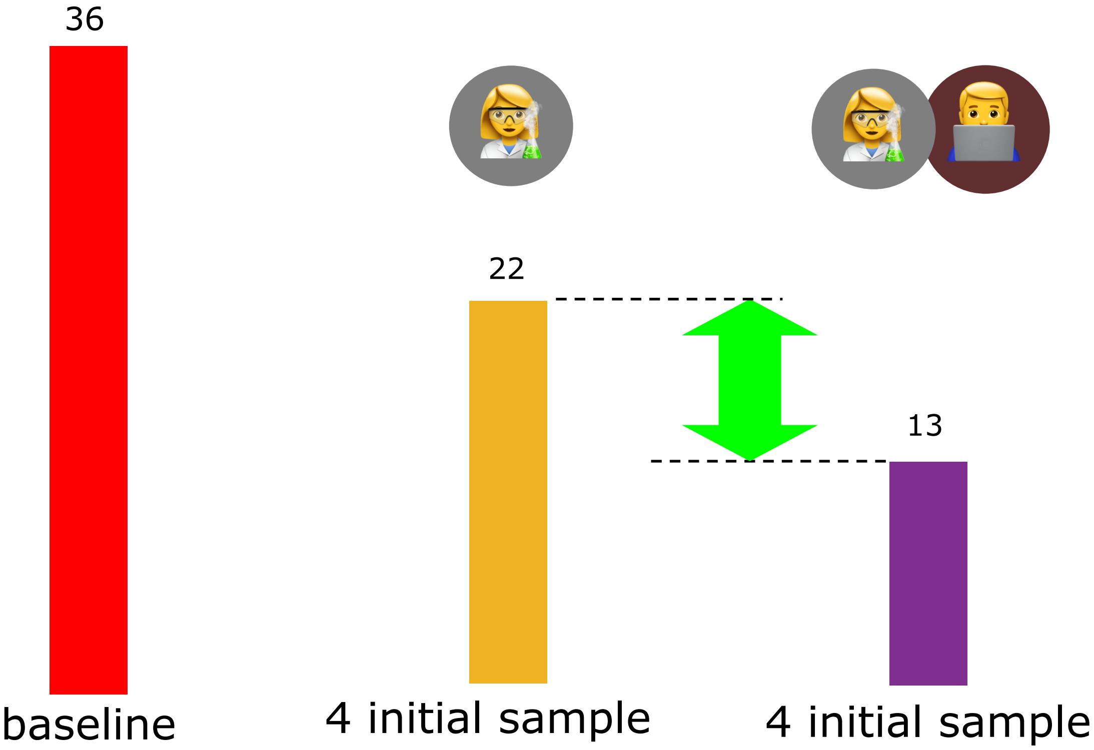
Q2: Training data



Mean required development cycle to reach top 5% performance with 90% certainty.

$$9\ data\ sets\ *$$
$$25\ randomized\ runs\ *$$
$$6\ algorithms\ =$$
$$\underline{\mathbf{1350}\ Experiments/Scenario}$$

Q3: Naïve vs. informed



Mean required development cycle to reach top 5% performance with 90% certainty.

$$9\ data\ sets\ *$$

$$25\ randomized\ runs\ *$$

$$6\ algorithms\ =$$

$$\underline{\mathbf{1350}\ \ Experiments/Scenario}$$

Performance in different scenarios

Mean development cycle to meet target with 90% certainty

		4 initial sample	20 initial sample
naive	👩‍🔬	22	16
informed	👩‍🔬 👨‍💻	13	10

Configuration decisions an their impact

Decision	**Best decision (requ. dev. cycle)**	**Alternative decision (requ. dev. cycle)**	**Improvement (requ. dev. cycle)**
Optimization target	Multi-objective (13.8)	Single-objective (22.2)	8.4
Model	Gauss Process (17.7) *(statistic model)*	Random Forrest (18.3) *(Machine Learning model)*	0.6
Pipeline	Vanilla + PCA (13.7)	Vanilla (23.5)	9.8
Strategy	Exploration (15)	Exploitation (20.9)	5.9
Initial sample size	20 (13.9)	4 (22)	8.1

General advice

1. Select prediction model

explores better

Statistics-based model (**Gaussian Process** regression, GP)

- when the material data is continuous and relatively low dimensional

predicts better,
but requires more data

AI model (**Random Forrest** regression, RF)

- when categorical descriptors (e.g. cement type)
- input space is not continuous, i.e. it contains completely different materials

General advice: Start with GP and try out RF if predictions are not satisfying

General advice

2. Adjust curiosity

<0 (exploit)

- when sufficient prediction data available (sufficient data + good model)
- when training data similar to candidates & models are certain
- when deadlines are pressing

0> (explore & exploit)

- to discover "moon-shot" materials (e.g. if predictions are not satisfying)
- at the beginning of experimentation and for long-term studies

General advice

3. four criteria for the selection of candidates

Criteria 1: **Utility**

- the higher the better
- multi-objective optimization: adjust weights to prioritize desired property combinations

Criteria 2: **Prediction & uncertainty**

- predicted materials properties desired?
- if exploiting: uncertainty tolerable?

General advice

3. four criteria for the selection of candidates

Criteria 3: **A-priori information** (only if applicable)

– does the candidate meet the requirements?

Criteria 4: **Novelty** (between 0 and 1)

- indicating the difference from the training data
- a relatively low novelty (e.g. 0.05) does not introduce major changes in the composition and might therefore receive a lower priority

General advice

3. four criteria for the selection of candidates

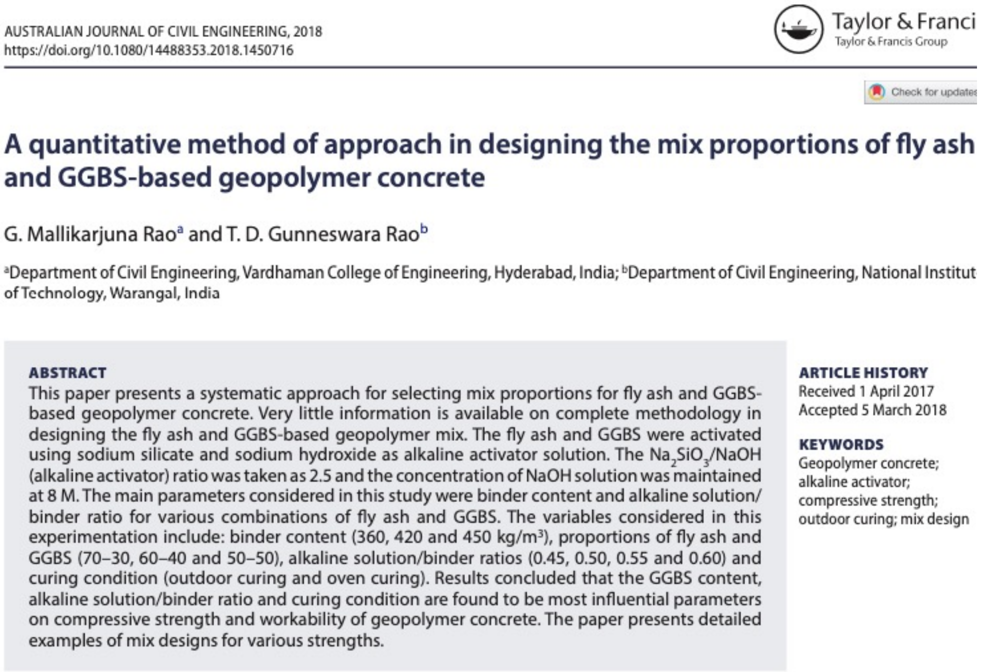
If criteria 1…4 do not provide satisfying results:

- try different model (GP vs. RF)
- adjust weights to change prioritization
- adjust curiosity to explore more (if only undesired materials predicted) or exploit more if good candidates already available

Design Task

www.bam.de

Geopolymer concrete parameters



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https://doi.org/10.1080/14488353.2018.1450716

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Check for update

A quantitative method of approach in designing the mix proportions of fly ash and GGBS-based geopolymer concrete

G. Mallikarjuna Rao[a] and T. D. Gunneswara Rao[b]

[a]Department of Civil Engineering, Vardhaman College of Engineering, Hyderabad, India; [b]Department of Civil Engineering, National Institut of Technology, Warangal, India

ABSTRACT
This paper presents a systematic approach for selecting mix proportions for fly ash and GGBS-based geopolymer concrete. Very little information is available on complete methodology in designing the fly ash and GGBS-based geopolymer mix. The fly ash and GGBS were activated using sodium silicate and sodium hydroxide as alkaline activator solution. The Na_2SiO_3/NaOH (alkaline activator) ratio was taken as 2.5 and the concentration of NaOH solution was maintained at 8 M. The main parameters considered in this study were binder content and alkaline solution/binder ratio for various combinations of fly ash and GGBS. The variables considered in this experimentation include: binder content (360, 420 and 450 kg/m³), proportions of fly ash and GGBS (70–30, 60–40 and 50–50), alkaline solution/binder ratios (0.45, 0.50, 0.55 and 0.60) and curing condition (outdoor curing and oven curing). Results concluded that the GGBS content, alkaline solution/binder ratio and curing condition are found to be most influential parameters on compressive strength and workability of geopolymer concrete. The paper presents detailed examples of mix designs for various strengths.

ARTICLE HISTORY
Received 1 April 2017
Accepted 5 March 2018

KEYWORDS
Geopolymer concrete; alkaline activator; compressive strength; outdoor curing; mix design

Design Parameters

Fly-ash/GGBFS ratio: 70-30, 60-40, 50-50

Alkaline solution/binder ratio: 0.45, 0.5, 0.55, 0.6

Admixture: Super plasticiser 4 wt. % of Binder

Curing: ambient/oven

Binder content: 360, 370, 380, 390,400, 410, 420, 430, 440, 450 kg

Constants:

Fine/coarse aggregate: 45 wt.% / 55 wt.%

Target: impact of the above on compressive strength

Task: Discover a powerful concrete recipe!

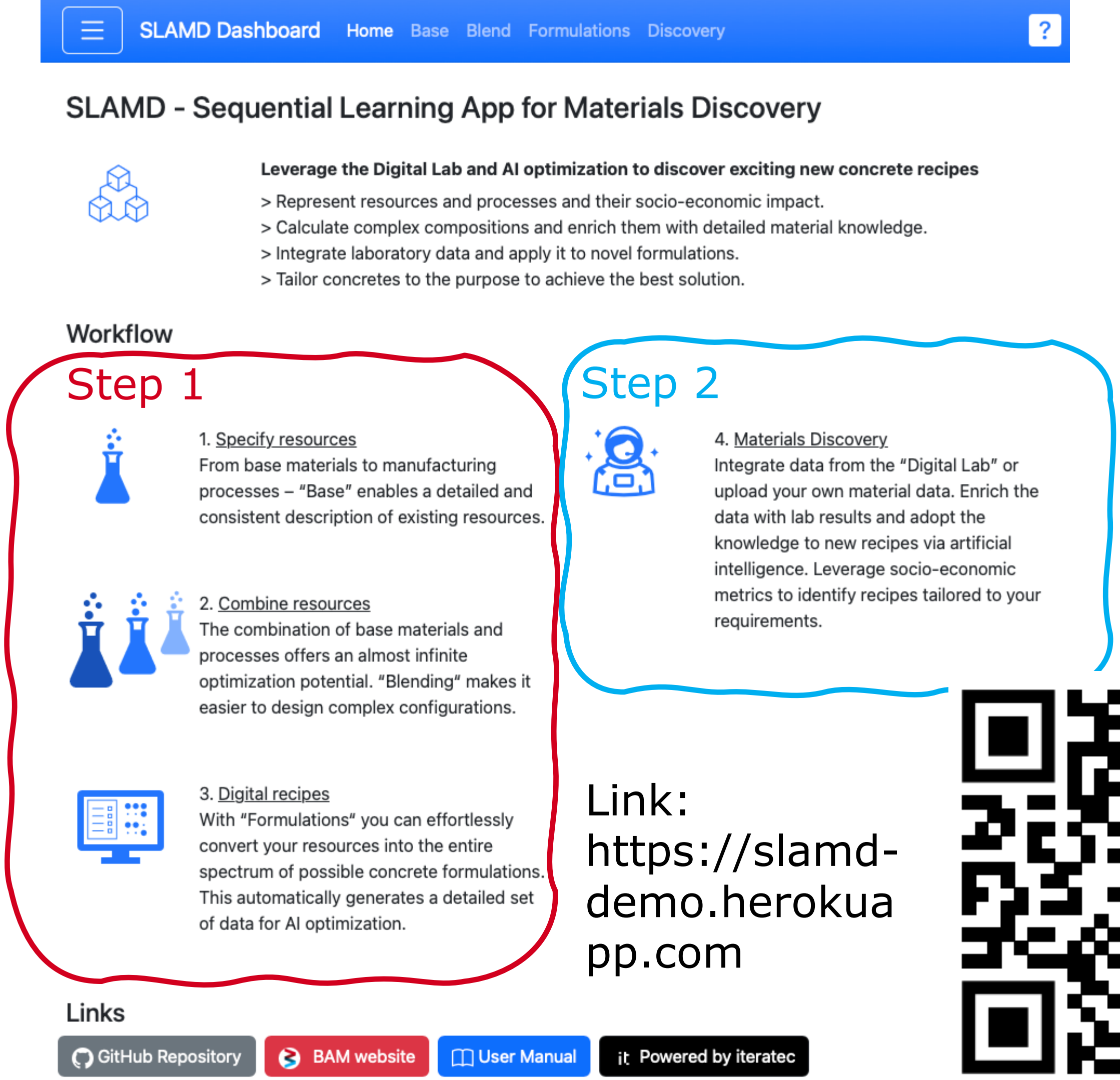
You get the instructions for a batch of 240 **geopolymer** concretes.

Step 1

- Create the formulations using SLAMD’s digital twin

Step 2

- given 10 laboratory validation data use the inverse design approach to find ideal formulations



SLAMD - Sequential Learning App for Materials Discovery

Leverage the Digital Lab and AI optimization to discover exciting new concrete recipes

> Represent resources and processes and their socio-economic impact.
> Calculate complex compositions and enrich them with detailed material knowledge.
> Integrate laboratory data and apply it to novel formulations.
> Tailor concretes to the purpose to achieve the best solution.

Workflow

Step 1

1. Specify resources
From base materials to manufacturing processes – "Base" enables a detailed and consistent description of existing resources.

2. Combine resources
The combination of base materials and processes offers an almost infinite optimization potential. "Blending" makes it easier to design complex configurations.

3. Digital recipes
With "Formulations" you can effortlessly convert your resources into the entire spectrum of possible concrete formulations. This automatically generates a detailed set of data for AI optimization.

Step 2

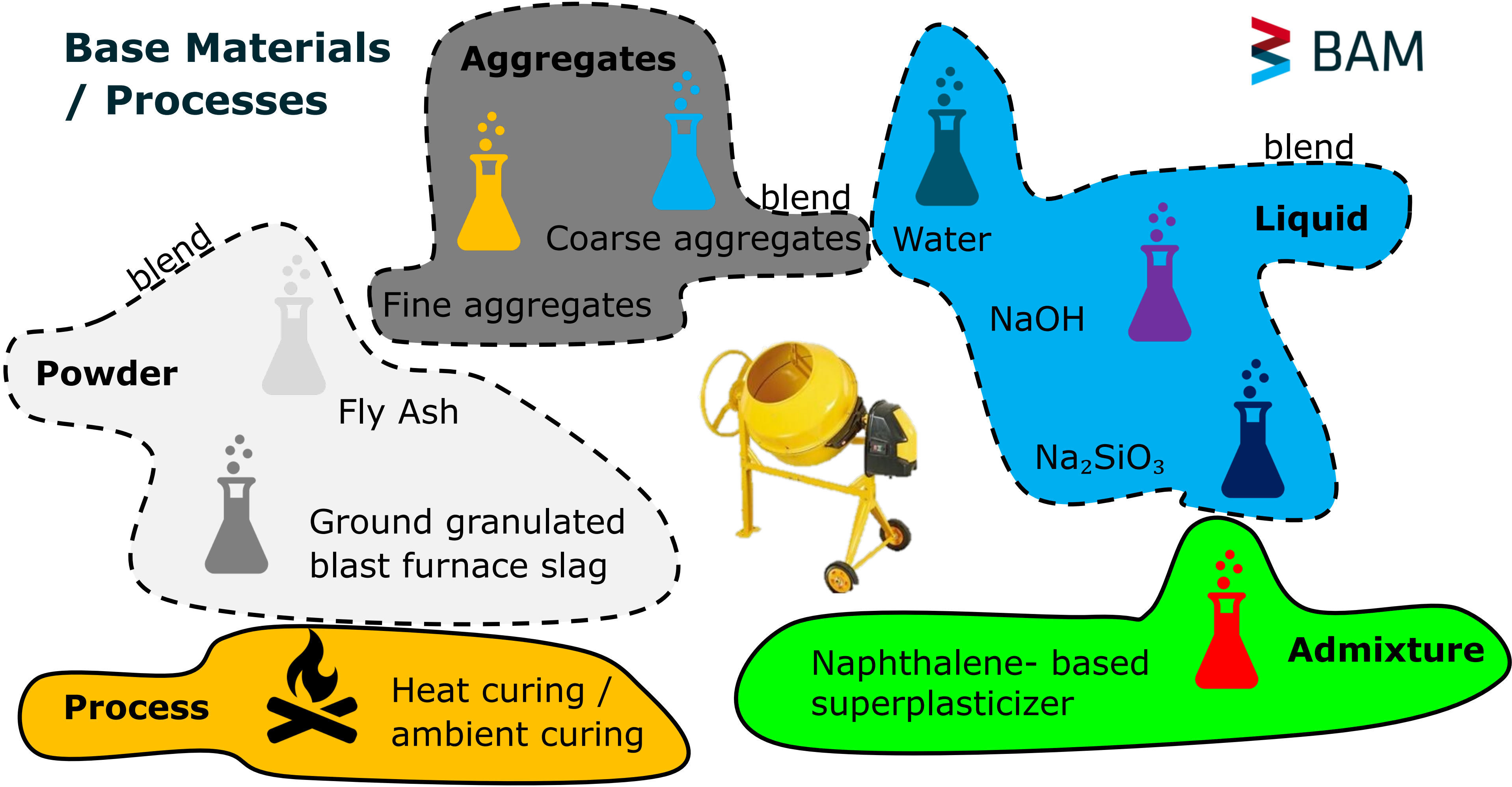
4. Materials Discovery
Integrate data from the "Digital Lab" or upload your own material data. Enrich the data with lab results and adopt the knowledge to new recipes via artificial intelligence. Leverage socio-economic metrics to identify recipes tailored to your requirements.

Links

Link: https://slamd-demo.herokuapp.com

Base Materials / Processes

BAM



Aggregates

Coarse aggregates

Fine aggregates

blend

Powder

Fly Ash

Ground granulated blast furnace slag

blend

Liquid

Water

NaOH

Na_2SiO_3

blend

Admixture

Naphthalene- based superplasticizer

Process

Heat curing / ambient curing

Base Materials - Powder

	Composition									**Cost**
	Fine modulus (m²/kg)	Fe_2O_3 (m%)	SiO_2 (m%)	Al_2O_3 (m%)	CaO (m%)	MgO (m%)	Na_2O (m%)	SO_3 (m%)	LOI (m%)	CO_2 footprint (kg/ton)
FA	380	4.25	60.11	26.53	4.0	1.25	0.22	0.35	3.25	4
GGBFS *	426	0.8	34.06	20.0	32.6	7.89	0.0	0.9	3.72	52.0

The example session file already contains some materials.
Materials with star „*“must be added in SLAMD.

Base Materials - Liquid

	Composition			**Cost**
	Na_2SiO_3 (m%)	NaOH (m%)	H_2O (m%)	CO_2 footprint (kg/ton)
Water	0	0	100	0
NaOH*	0	100	0	1915.0
Na_2SiO_3	100	0	0	360.0

The example session file already contains some materials.
Materials with star „*“must be added in SLAMD.

Base Materials - Aggregates

	Composition						**Cost**
	Fine Aggregates (m%)	Coarse Aggregates (m%)	Specific gravity (kg/m³)	Bulk density (kg/m³)	Fineness modulus (m³/kg)	Water absorption (m%)	CO_2 footprint (kg/ton)
Fine	100	0	2.65	1.45	2.57	2.0	4.8
Coarse	0	100	2.8	1.5	7.3	0.5	4.8

Base Materials - Admixture

Cost

	CO_2 footprint (kg/ton)
Sulphonated Naphthalene formaldehyde-based superplasticizer *	1880

The example session file already contains some materials.
Materials with star „*"must be added in SLAMD.

Process - Curing

	Process Information		Cost
	Duration (days)	Temperature (°C)	CO_2 footprint (kg)
Heat*	1	60	22.45
Ambient	1	25	0

The example session file already contains some materials.
Materials with star „*“must be added in SLAMD.

Blends

Powders (3): FA / GGBFS
50 / 50
60 / 40
70 / 30

Liquid (1): H_2O / NaOH / Na_2SiO_3
72 / 8 / 20

Aggregates (1): Fine / Coarse
40 / 60

Formulation

(# of variations) Design Parameters

(3) Fly-ash/GGBFS ratio: 70-30, 60-40, 50-50

(4) Alkaline solution/binder ratio: 0.45, 0.5, 0.55, 0.6

(1) Admixture: Super plasticiser 4 wt. % of Binder

(2) Curing: ambient/oven

(10) Binder content: 360, 370, 380, 390,400, 410, 420, 430, 440, 450 kg

(1) Fine/coarse aggregate: 45 wt.% / 55 wt.%

3 x 4 x 1 x 2 x 10 -> **240 Formulations**

Constraint (Sum of materials used for formulation) = 2400 kg ~ **1m^3**

Design Tasks

1. Single-objective

Target = *high strength*

$$f_{c(28d)} > 61.94\,MPa \quad (5\% \;-\!> 12/240)$$

2. Multi-objective

Target = *high strength & climate friendly*

$$f_{c(28d)} > 50\,MPa$$

$$CO_2 < 85\,kg/m^3 \quad (5\% \;-\!> 12/240)$$

Questions?

BAM

“SLAMD” - Sequential Learning App for Materials Discovery

Repository: https://github.com/BAMresearch/WEBSLAMD

Case Studies

Völker et al. 2022, http://dx.doi.org/10.13140/RG.2.2.33502.92480/1

Völker et al. 2021, http://dx.doi.org/10.13140/RG.2.2.18388.94087/1

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