Technische Universität Berlin

BAM Bundesanstalt für Materialforschung und -prüfung

Sicherheit in Technik und Chemie

25.01.2024

DATA DRIVEN MATERIALS DESIGN PART III.

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1

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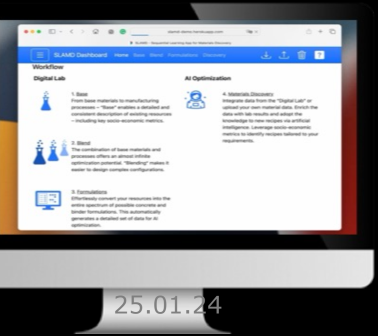

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Scope

1. Introduction to data driven materials design (last week)
   - Digital materials
   - Predicting properties
   - Decision making
2. **Prospects of LLMs**
3. Hands on (next week)
   - AI-driven materials design
     - SLAMD
     - LLM

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

SLAMD Workflow

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SLAMD Dashboard Home Base Blend Formulations Discovery ?

BAM

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

1. 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.

2. AI-Optimization

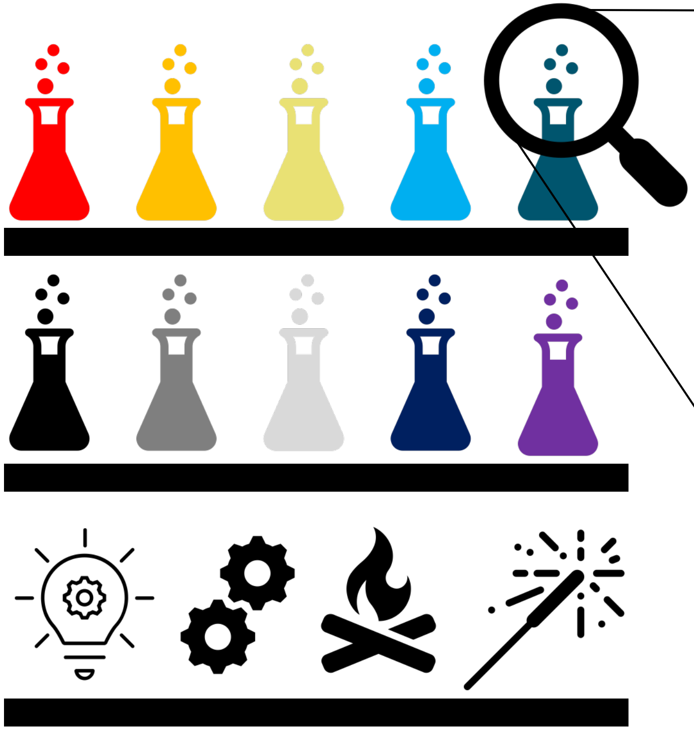
4. Materials Discovery
Integrate data from the “Digital Lab” or upload your own material data. Enrich the data with lab results and adopt the knowledge to new recipes via artificial intelligence. Leverage socio-economic metrics to identify recipes tailored to your requirements.

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

Links

GitHub Repository | BAM website | User Manual | it Powered by iteratec

Digital Lab



Digital Twin

Materials prop.

.........% CaO

.... % SiO_2

.... mm^2/g

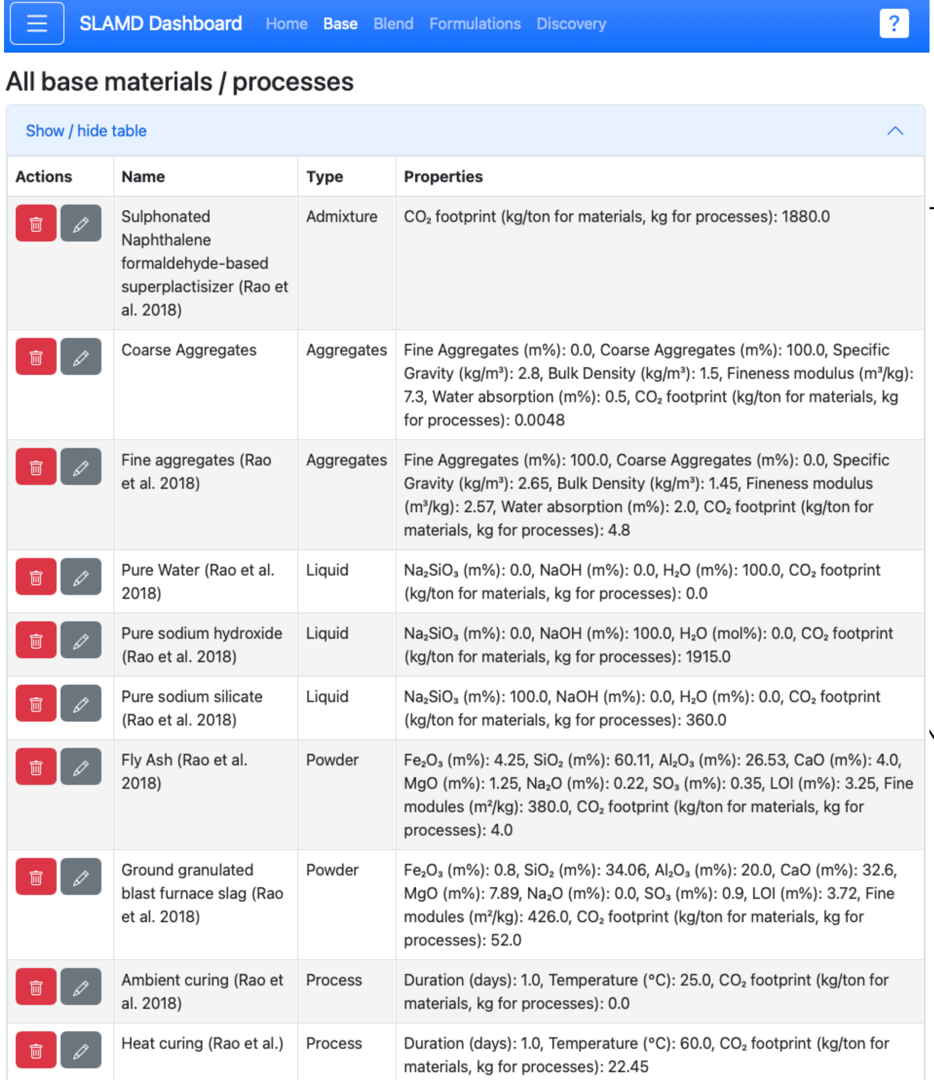
....

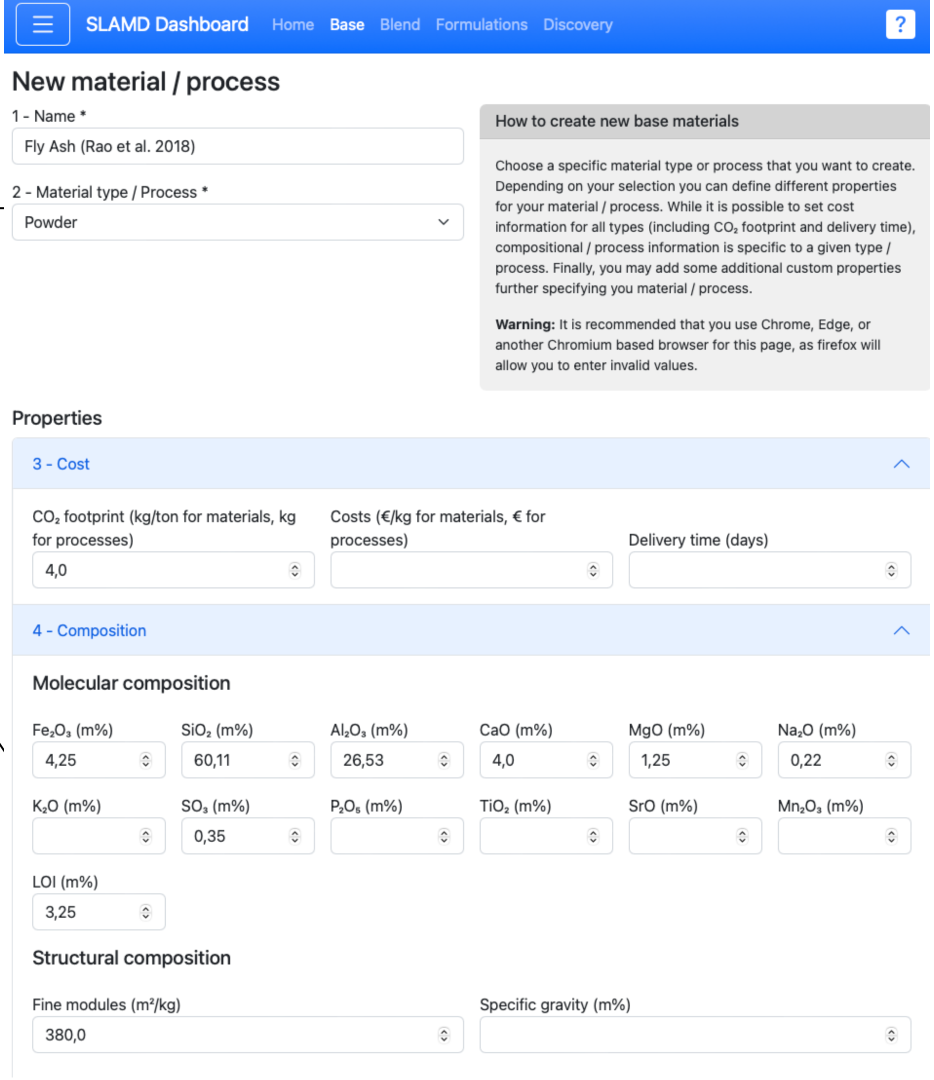
Socio-eco. prop.

.... $kgCO_2$

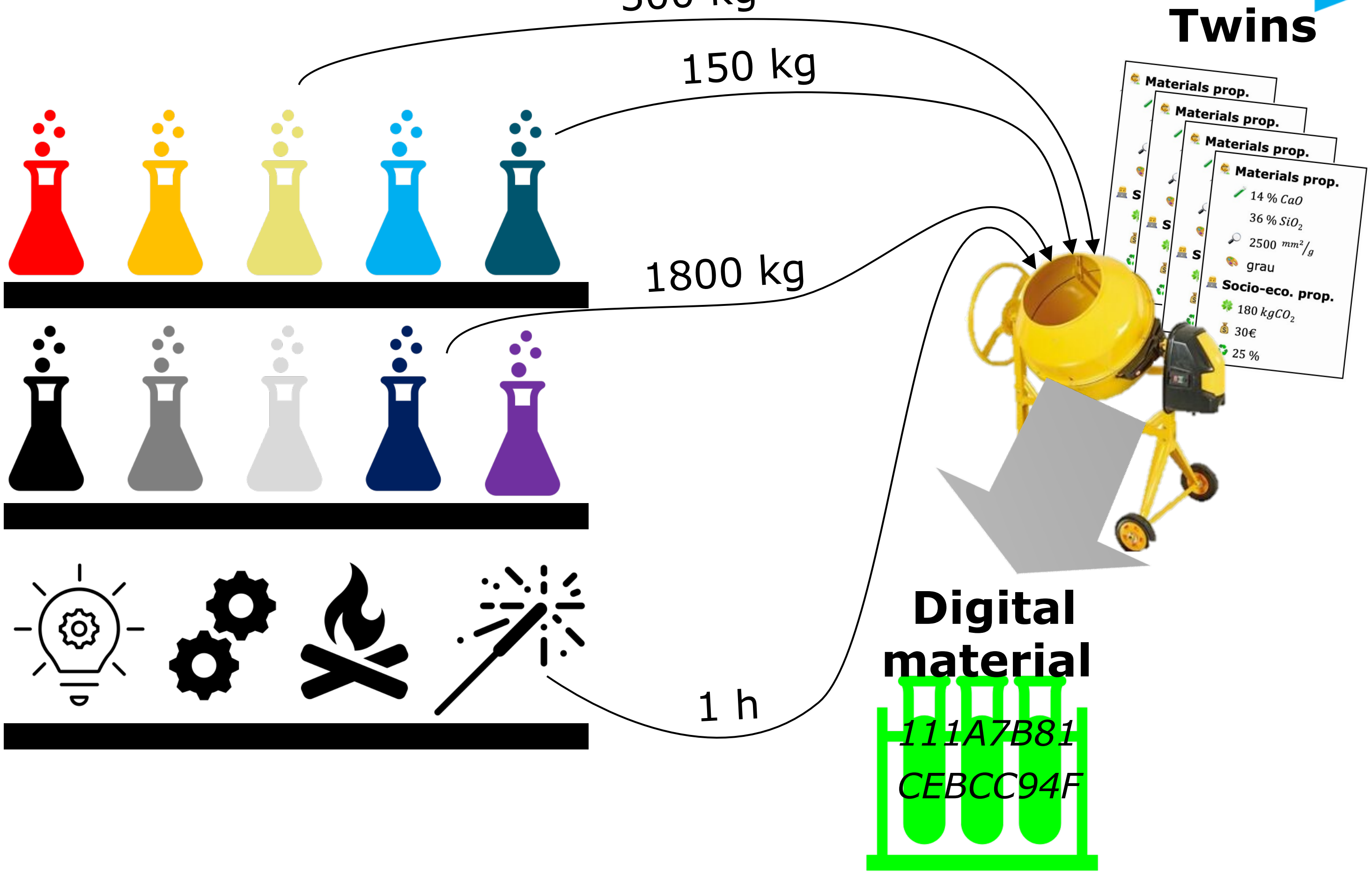
.... €

.... %


SLAMD Dashboard
Home
Base
Blend
Formulations
Discovery
?
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

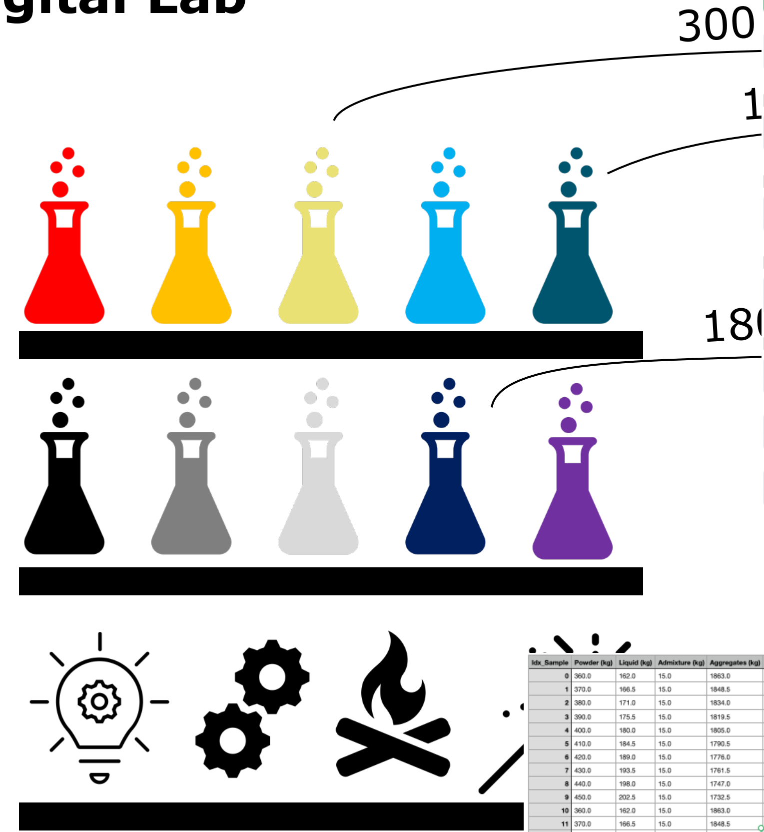

SLAMD Dashboard
Home
Base
Blend
Formulations
Discovery
?
New material / process
1 - Name *
Fly Ash (Rao et al. 2018)
2 - Material type / Process *
Powder
How to create new base materials
Choose a specific material type or process that you want to create. Depending on your selection you can define different 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%)

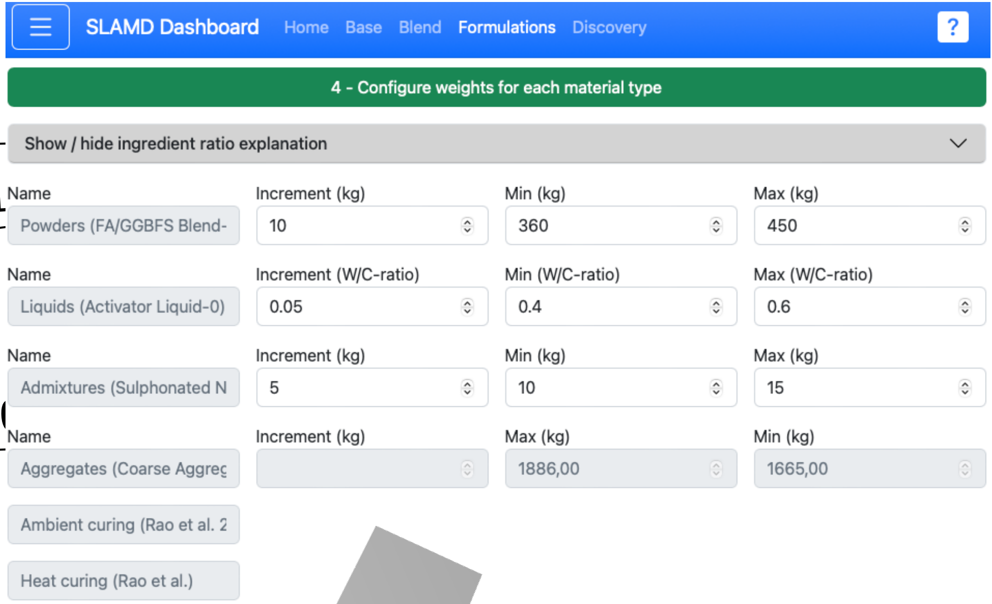
Digital Lab

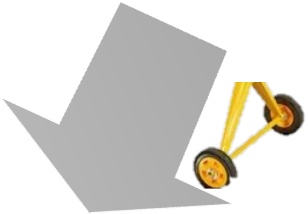


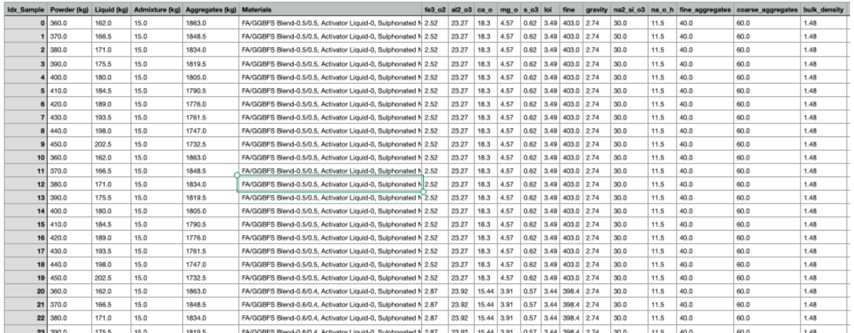
300 kg
150 kg
1800 kg
1 h
Digital Twins
Materials prop.
14 % CaO
36 % SiO2
2500 mm²/g
grau
Socio-eco. prop.
180 kgCO2
30€
25 %
Digital material
111A7B81
CEBCC94F

Digital Lab





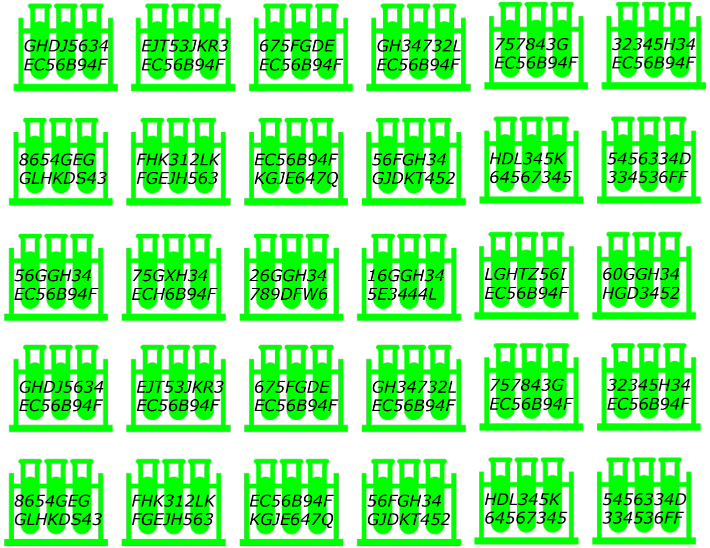




Idx_Sample	Powder (kg)	Liquid (kg)	Admixture (kg)	Aggregates (kg)	Materials	fe3_o2	al2_o3	ca_o	mg_o	s_o3	loi	fine	gravity	na2_si_o3	na_o_h	fine_aggregates	coarse_aggregates	bulk_density
0	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	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
23	390.0	175.5	15.0	1819.5	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

AI Optimization - Materials discovery dashboard

Import materials search space



Set objectives

Strenght (Maximize)

Threshold: 45 MPa

Costs (Minimize)

Threshold: 90 €

CO_2-Footprint (Minimize)

Threshold: 120 kg/ton

SLAMD Dashboard Home Base Blend Formulations **Discovery**

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

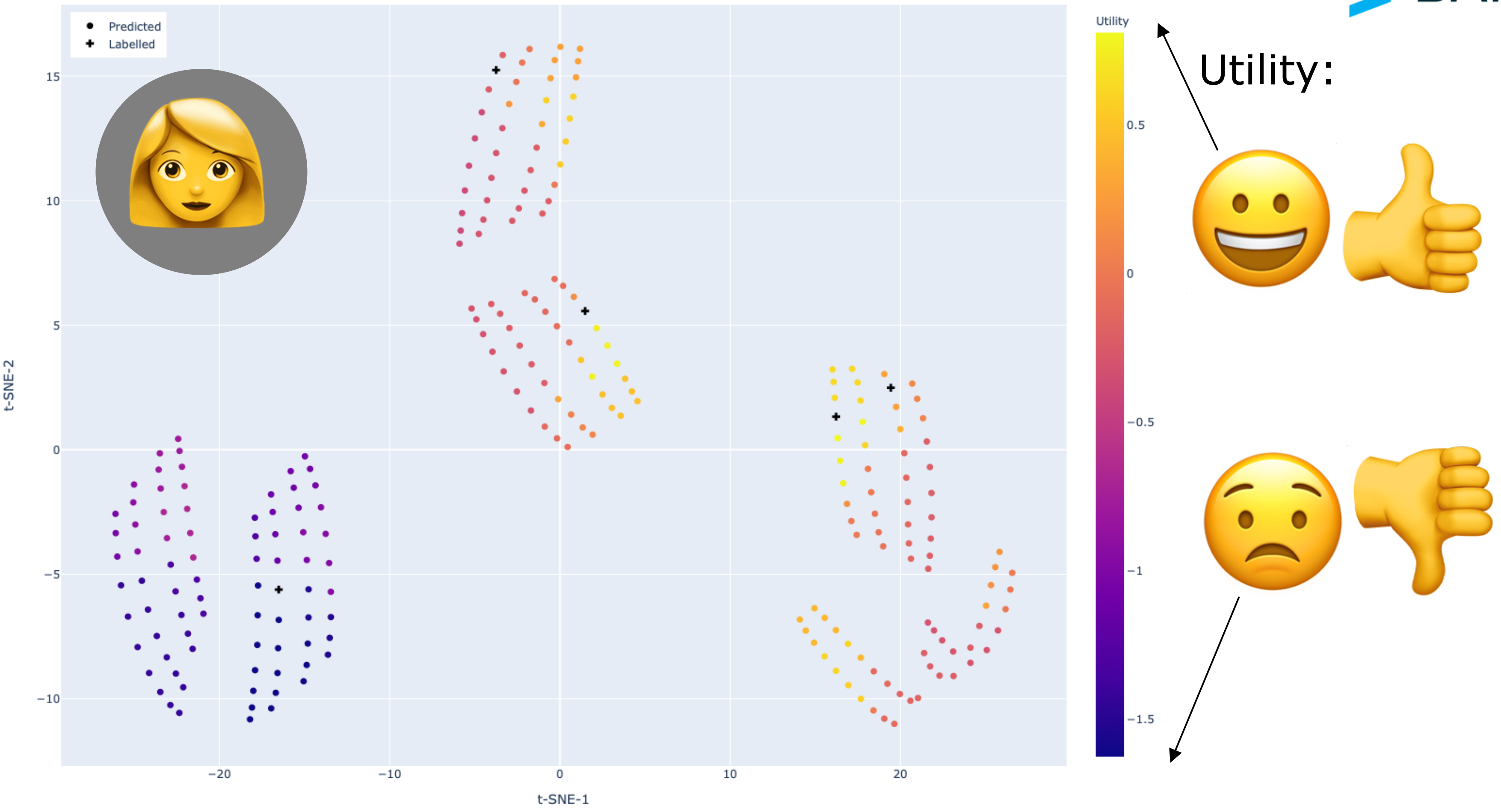
A priori Information (optional)

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



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

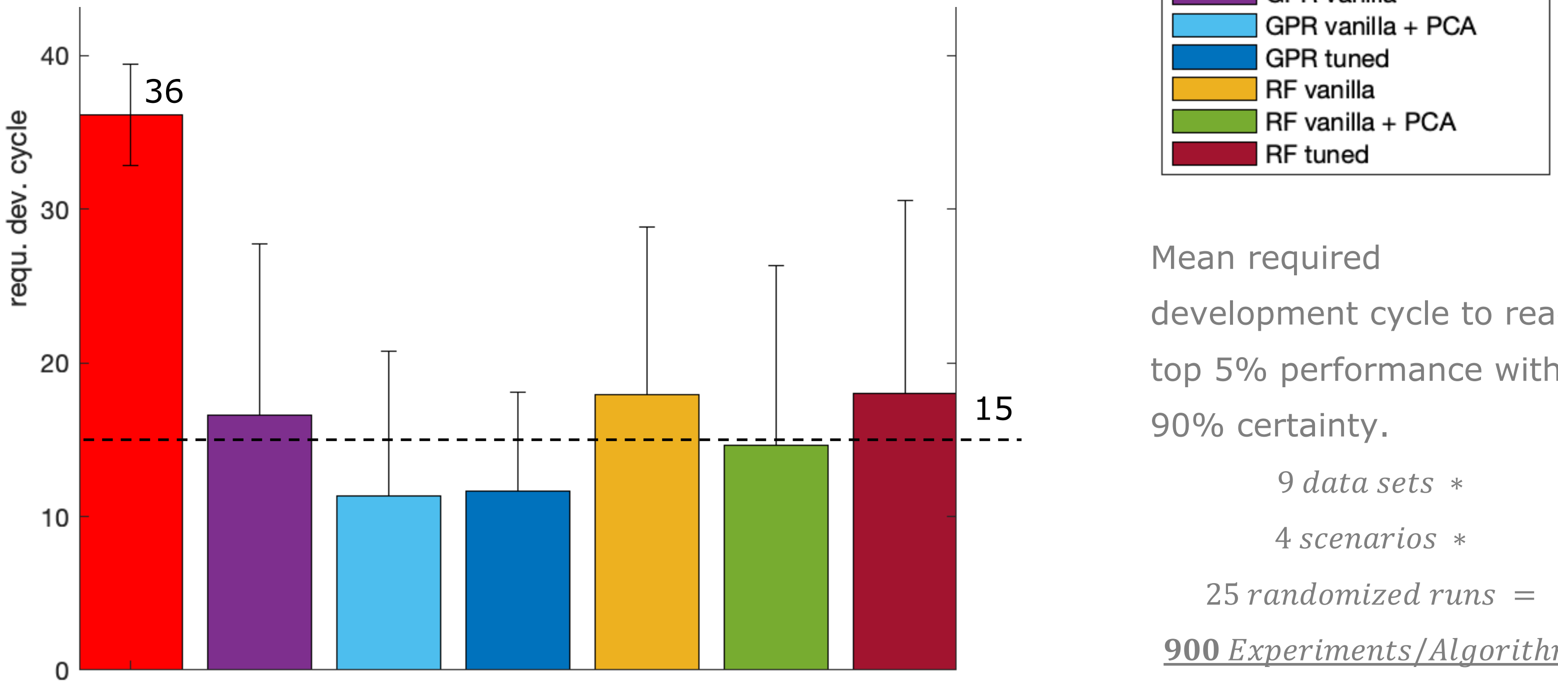
compressive strength (MPa)

CO_2 footprint (kg/ton)

Benchmarking (required development cycle)

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

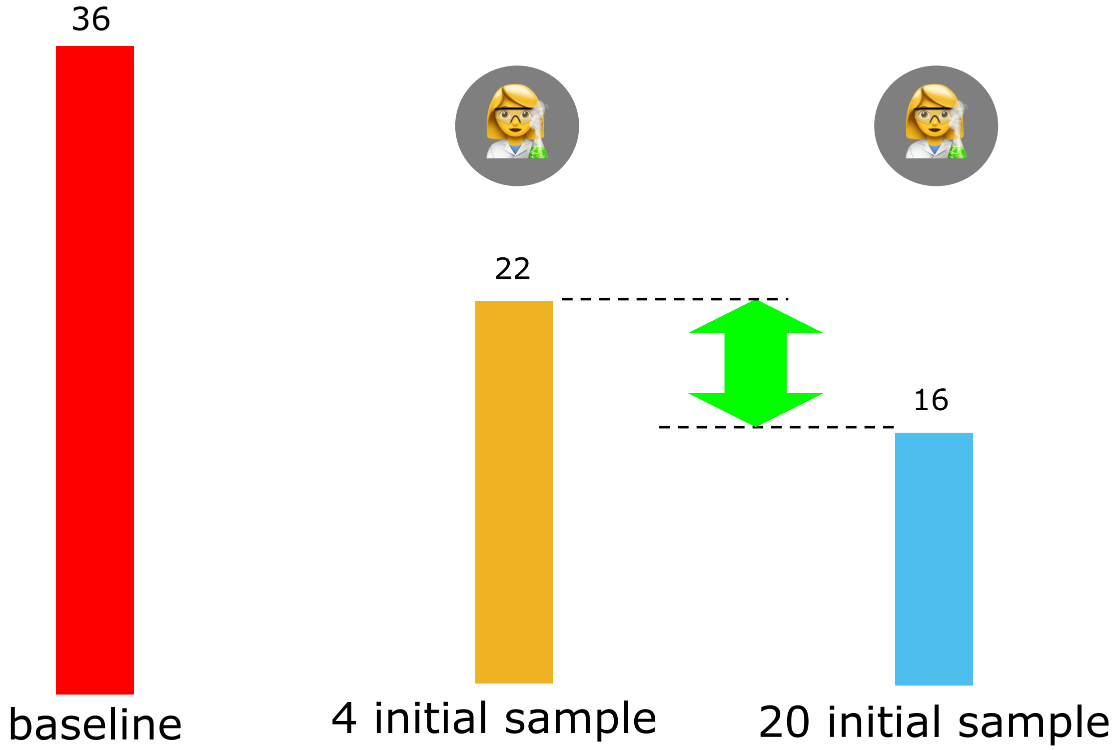
Q1: Algorithm



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

$$9\ data\ sets\ *$$
$$4\ scenarios\ *$$
$$25\ randomized\ runs\ =$$
$$\underline{\mathbf{900}\ Experiments/Algorithm}$$

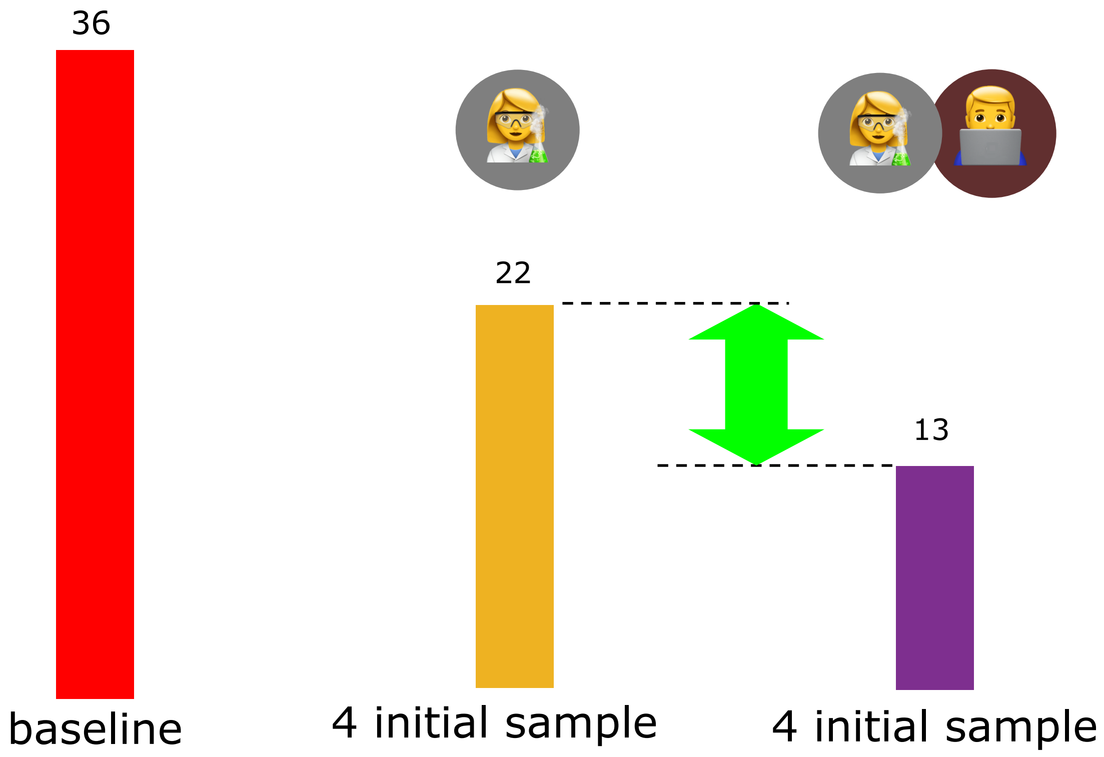
Q2: Training data



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

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Geopolymer concrete parameters

BAM

AUSTRALIAN JOURNAL OF CIVIL ENGINEERING, 2018
https://doi.org/10.1080/14488353.2018.1450716

Taylor & Franci
Taylor & Francis Group

Check for updates

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

Design Parameters

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

W/C: 0.45, 0.5, 0.55, 0.6

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

Curing: ambient/oven

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 Dashboard Home Base Blend Formulations Discovery ?

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.

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

Links

GitHub Repository | BAM website | User Manual | Powered by iteratec

Base Materials / Processes

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 (m^2/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*

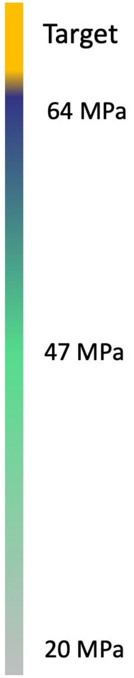
$f_{c(28d)} > 50\,MPa$

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

Hands on!

Ground Truth Data

Blend	Curing	W/C	Powder Content - (kg)									
			360	370	380	390	400	410	420	430	440	450
50/50	Ambient	0,45	55,4	55,6	55,9	56,1	56,4	56,6	56,9	54,1	51,9	48,9
		0,5	59,8	59,9	60,0	60,1	60,2	60,3	60,4	59,8	59,2	58,5
		0,55	51,6	50,7	49,9	49,0	48,1	47,3	46,5	47,2	47,7	48,5
		0,6	46,7	46,8	47,0	47,1	47,3	47,4	47,6	47,6	47,6	47,6
	Heat	0,45	62,0	61,2	60,5	59,7	59,0	58,2	57,5	56,7	55,8	55,0
		0,5	**65,3**	**65,1**	**64,9**	64,8	64,6	64,4	64,3	63,5	62,7	61,9
		0,55	53,4	52,9	52,5	52,0	51,5	51,1	50,6	51,9	53,2	54,4
		0,6	52,4	51,9	51,4	50,9	50,4	49,9	49,4	50,9	52,4	53,8
60/40	Ambient	0,45	43,3	43,0	43,6	44,2	44,9	45,5	46,1	46,0	46,0	45,9
		0,5	47,9	48,5	47,9	48,8	49,6	50,4	51,2	51,0	50,9	50,7
		0,55	46,9	46,5	46,1	45,8	45,4	45,0	44,7	43,7	42,9	41,9
		0,6	43,4	46,2	46,3	46,4	46,4	46,5	46,6	46,3	46,0	45,7
	Heat	0,45	55,6	56,1	56,7	57,2	57,8	58,3	58,8	58,0	57,3	56,6
		0,5	57,4	58,2	59,0	59,9	60,7	61,5	62,3	62,0	61,6	61,3
		0,55	53,4	54,3	55,3	56,2	57,1	58,1	58,9	57,4	55,8	54,4
		0,6	51,2	52,1	53,1	54,0	54,9	55,8	56,6	54,3	52,0	49,8
70/30	Ambient	0,45	33,8	34,3	34,8	38,3	35,8	36,2	36,7	35,7	34,9	33,8
		0,5	36,2	36,5	36,9	37,2	37,5	37,9	38,2	38,4	38,7	39,0
		0,55	31,1	30,3	29,4	28,6	27,8	27,0	26,2	26,0	25,9	25,7
		0,6	25,7	25,6	25,5	25,4	25,3	25,2	25,1	23,6	22,4	20,8
	Heat	0,45	41,5	41,3	41,2	41,0	40,8	40,6	40,4	39,8	39,2	38,6
		0,5	42,6	42,7	42,9	43,0	43,2	43,4	43,5	43,8	44,2	44,5
		0,55	33,9	33,5	33,0	32,6	32,1	31,7	31,2	32,6	34,0	35,2
		0,6	25,6	28,3	28,0	27,7	27,4	27,2	26,9	27,8	28,7	29,5



Questions?

"SLAMD" - Sequential Learning App for Materials Discovery

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

Resources:

https://github.com/BAMresearch/WEBSLAMD#documentation

- Video Tutorial
- Benchmarking Paper
- Data Sets
- GPT-4 powered SLAMD Assistant