Beyond Theory: Pioneering AI-Driven Materials Design in the Sustainable Building Material Lab

Preprint · February 2024

DOI: 10.13140/RG.2.2.27019.67365

9 authors, including:

Christoph Völker
Bundesanstalt für Materialforschung und -prüfung
33 PUBLICATIONS **181** CITATIONS
SEE PROFILE

Elisabeth John
Bundesanstalt für Materialforschung und -prüfung
15 PUBLICATIONS **322** CITATIONS
SEE PROFILE

Rafia Firdous
Technische Universität Berlin
39 PUBLICATIONS **371** CITATIONS
SEE PROFILE

Tamino Hirsch
Technische Universität Berlin
32 PUBLICATIONS **501** CITATIONS
SEE PROFILE

Spring Convention & conference on
advanced construction materials and processes for a carbon neutral society
10-12 April 2024, Milan, Italy

BEYOND THEORY: PIONEERING AI-DRIVEN MATERIALS DESIGN IN THE SUSTAINABLE BUILDING MATERIAL LAB

Christoph Völker[1)], Elisabeth John[2)], Rafia Firdous[3)], Tamino Hirsch[4], Daria Kaczmarek[5)], Kevin Ziesak[5)], Anja Buchwald[6)], Dietmar Stephan[7)], Sabine Kruschwitz[8)]

[1] Dr. Ing., Bundesanstalt für Materialforschung und -prüfung, Germany, christoph.voelker@bam.de
[2] Dr. rer. nat., Bundesanstalt für Materialforschung und -prüfung, Technische Universität Berlin, Germany, elisabeth.john@bam.de
[3] Dr. Ing., Technische Universität Berlin, Germany, rafia.firdous@tu-berlin.de
[4] M. Sc., Technische Universität Berlin, Germany, t.hirsch@tu-berlin.de
[5] Technische Universität Berlin, Germany
[6] Dr. Ing., ASCEM B.V., Netherlands
[7] Prof. Dr. rer. nat., Technische Universität Berlin, Germany, stephan@tu-berlin.de
[8] Prof. Dr. rer. nat., Bundesanstalt für Materialforschung und -prüfung, Technische Universität Berlin, Germany, sabine.kruschwitz@bam.de

ABSTRACT

This work focuses on Artificial Intelligence (AI)-driven materials design, addressing the challenge of improving the sustainability of building materials amid complex formulations. These formulations involve various components, such as binders, additives, and recycled aggregates, necessitating a balance between environmental impact and performance. Traditional experimental methods often fall short in managing the complexity of material composition, hindering fast enough development of optimal solutions. Our research explores complex composition materials design through a comprehensive, comparative lab study between Data-Driven Design, using SLAMD - an open-source AI materials design tool, and traditional Design of Experiments (DOE). We aimed to develop a high-performance, alkali-activated material using secondary precursors, aiming for a compressive strength exceeding 100 MPa after 7-days. The findings reveal that AI-driven design outperforms DOE in development speed and material quality, successfully identifying multiple high-performance materials. This result showcases AI's capability to handle complex designs with limited data, marking a significant improvement over conventional methods and demonstrating AI's revolutionary role in sustainable material design. Our study provides in-depth insights into the real-world application of data-driven design in a laboratory setting, highlighting the effective collaboration between AI-guided design and expert oversight. By showcasing the successful integration of AI, this research contributes to advancing sustainable materials science. It sets the stage for shorter time-to-market development boosting the impact of sustainable building in the construction industry.

Keywords: *Data-Driven Design, Sequential Learning, Design of Experiments, Alkali-Activated Binder, Secondary Raw Materials,*

Sabine Kruschwitz, Prof. Dr. rer. nat.

Unter den Eichen 87, 12205 Berlin

Email: sabine.kruschwitz@bam.de | **Tel:** +49 30 8104-1442 | **Web:** www.bam.de

1. INTRODUCTION

The growing need to protect the environment and achieve the United Nations Sustainable Development Goals (SDGs), especially Goal 12: Responsible Consumption and Production, requires a reduction in the consumption of primary resources while increasing the use of secondary resources. This includes building materials of inorganic binders to produce mortar and concrete. To achieve the SDGs, the composition of inorganic binders is evolving towards significantly more complex mix designs. One reason is the increased number of (secondary) components; however, the compositional variability of the secondary raw materials is an additional challenge, as it is associated with less reliable chemical and physical properties inherited from their production processes.

One promising class of inorganic binders for future large-scale applications are alkali-activated materials (AAM). What makes them particularly promising is the fact that these binders can be produced from secondary resources, “wastes”. AAMs may achieve similar mechanical and durability properties as Ordinary Portland Cement (OPC) while emitting up to 80 % less CO_2 [1]. However, these benefits can only be achieved by the optimizing the composition of the mix design. The wide variety of solid precursors, typically a solid aluminum silicate, as well as alkaline solutions results in a large variability of the materials and their properties. Slags, fly ashes, clays, and natural stones are the most studied suitable solid precursors for alkaline activation, but numerous other industrial by-products and natural materials are suitable [2]. The use of industrial slags is most appropriate as they are produced in large quantities with comparatively less compositional variation [3]. The circular use of these large quantities is a major contribution to SDG 12. Each constituent affects the mix, strength or durability, and their interactions add a layer of complexity, creating an intricate optimization challenge. Reliable material performance is a key element for large-scale marked implementation, but errors in the mix design can result in reduced material properties or even binder degradation [4, 5, 6].

Due to the lack of digital tools that can handle such complex systems, mix design is typically based on the know-how of the skilled workers. Traditional mix design methods cannot handle this complexity, consequently, so more systematic approaches can be beneficial to accelerate the process and reduce the need for skilled laboratory personnel. Such computational approaches include Design of Experiments (DOE) and Artificial Intelligence (AI).

1.1. Points of Departure

In concrete science predictive machine learning (ML) applications have been widely investigated, typically with a focus on the accuracy of predicted material properties [7, 8, 9]. Complementary, data-driven design (DDD) methods exploit predictive models with a focus on discovering promising material compositions. This has been demonstrated for several classes of materials [10]. The efficiency of these methods is often benchmarked through simulated experiments in which the outcomes of possible designs are predetermined. This allows the

evaluation of the DDD to identify desired materials under random initial conditions, as statistically analyzed by Ling et al. [11].

Research by Golafshani et al. [12], Zhang et al. [13], and Shobeiri et al. [14] has focused on the design of eco-friendly concrete mixes using generative design and genetic algorithms. While these approaches suggest new, promising compositions, they require large datasets (~1000 data points), making data collection both expensive and time consuming, especially for precursors with varying compositions.

Völker et al. [15] showed that DDD is highly efficient for cementitious materials, outperforming traditional ML methods with substantial fewer data points required to guide the design of complex materials. This study not only underlined ML's potential in the building materials sector but also its practical relevance and efficiency in data visualization. Völker et al. [16] further investigated impacting factors of DDD for the development of sustainable building materials in a large-scale study with more than 10,000 virtual experiments across nine AAM data sets – deriving clear guidance for application DDD. This work led to the development of SLAMD (Sequential Learning App for Materials Discovery), a DDD software for cementitious materials making this innovative design method accessible in the laboratory [17].

1.2. Research Gap, Hypothesis, and Research Question

While statistical benchmarking and methodological advancements present valuable insights, they underscore a critical research gap: the practical translation of these theoretical potentials into tangible outcomes in laboratory settings. We hypothesize that the application of DDD methodologies can substantially accelerate the experimental development process. To investigate this proposition, our study is centered around the following research questions (RQ):

RQ 1: How do the methodologies of DOE and AI contribute to a more rapid and efficient mix design for AAM?

RQ 2: To what extent can these two design approaches, individually and in comparison, enhance the progress and final quality of mix designs for AAM?

Our goal is to critically assess the impact of the AI-driven design strategy on formulating sustainable material compositions. The results will be benchmarked against the already stablished materials design by DOE. This evaluation aims to bridge the theoretical and practical realms, offering insights that advance the field of sustainable materials science.

2. MATERIALS & METHODS

2.1. Materials

The alkali-activated binders of the study were based on an industrial glass precursor. Table 1 shows its chemical composition. This glass was mixed with several sodium-based activator solutions that will be specified in section 3. The composition and quantity of these activator solutions was determined and optimized by DOE and AI.

Table 1: X-ray fluorescence analysis of the glass precursor used in this work.

	Al_2O_3	CaO	Cr_2O_3	Fe_2O_3	K_2O	MgO	Mn_2O_3	Na_2O	SiO_2	SO_3	TiO_2
M.-%	18.5	41.6	0.6	1.4	0.2	6.3	0.3	0.9	28.3	0.8	0.6

2.2. Data-Driven Design vs. Design of Experiments

While both, DDD and DOE aim to streamline the development process of materials, their methodologies, underlying principles, and effectiveness in handling complexity differ significantly.

DDD embodies an AI-enhanced methodology that systematically explores a vast array of material combinations and processing parameters through the creation and navigation of a design space (DS). This DS is an extensive table that contains all conceivable material formulations, enabling the consideration of a broad spectrum. The strength of DDD lies in its ability to embrace the complexity of material design without the constraints typically imposed by traditional experimental frameworks. This is achieved by utilizing predictive models (e.g., from machine learning) to transfer limited knowledge from an initial dataset to uncharted areas of the DS. This search process, where the most promising materials are sought after, is iterative: cycles of exploration (to maximize knowledge by delving into areas of uncertainty) are followed by final exploitation (to leverage accumulated knowledge in areas where the model predicts high potential). The method targets formulations meeting set performance criteria, allowing tailored material discovery.

Conversely, **DOE** is a more traditional method that seeks to optimize processes or mixtures through a structured experimental plan. This approach generates a model of the entire design space in a first step and then predicts optimized mixtures based on that model. Common DOE focuses on quadratic relationships to understand non-linear interactions between factors. However, DOE's effectiveness diminishes in the face of complex material compositions where the interactions between components are not well understood or are highly non-linear. The method relies on predefining factor levels and assumes interactions can be captured by the experimental plan.

The main differences between DDD and DOE in approaching a design task lie in their handling of the design target: DDD uses AI to learn from experimental data, focusing on the design

target. This allows it to navigate through complex interactions, optimizing formulations effectively. In contrast, DOE systematically explores the design space using predefined plans, lacking feedback from the design target until the final model is generated.

3. SAMPLE PREPARATION AND EXPERIMENTS

The experimental parameters of this study are summarized in Table 2 and are described in the following.

Table 2: Experimental parameters

No.	Parameter		Description
1)	Target		7-day compressive strength >100 MPa
2)	Sample size		20 x 20 x 20 mm^3
3)	Implementation		DOE: Minitab; DDD: SLAMD
4)	Lab budget		Max. 50 formulations in max 12 weeks
5)	Activator compounds:	Na-silicate [g]	0 – 122.2
		Na_2SO_4 [g]	0 – 91.7
		Na_2CO_3 [g]	0 – 6.4
		NaOH [g]	0 – 51.6
		W/S [g/g]	0.5 – 0.6

1) The target of this study was to find high performance materials that exceed a 7-day compressive strength of 100 MPa. **2)** The pastes were cast as 2 cm^3 cubes and vibration compacted. Sample preparation and seal curing were performed at 20 °C to exclude moisture loss and carbonation. The activator solutions were premixed one day earlier to release dissolution heat. **3)** The designs were carried out using the software SLAMD [17] for the DDD and Minitab for DOE. **4)** Due to the intensive labor and time required for quality assurance, the study was constrained to testing a maximum of 50 samples within a 12-week period. Quality assurance protocols necessitated the production of six samples for each formulation at test ages of 1, 7, and 28 days, resulting in a total of 18 samples per formulation and cumulatively amounting to 900 lab tests for a 50-formulation run. **5)** The study explored varying proportions of sodium-based activators: hydroxide, sulphate, carbonate, and silicate, each contributing up to a maximum of 40 grams of sodium oxide equivalent. The sodium silicate used in the formulations had a specific composition of 14.7% Na_2O, 30.2% SiO_2, and 55.1% H_2O by weight.

3.1. Experimental Procedure for Data-Driven Design with SLAMD

The procedure can be delineated into three steps: the initial preparation of the design space, the collection of training data, and the systematic exploration and optimization of material formulations across seven development cycles.

1) The construction of the DS began with the variation of each constituent in 10% intervals,

ranging from 0% to 100%. Additionally, the water-to-solids (W/S) ratio was varied across three discrete values: 0.5, 0.55, and 0.6. This variation was automated using an Excel tool, culminating in a DS that included 43,923 potential formulations, encapsulating all conceivable activator combinations.

2) For the initial training set 6 formulations were strategically selected to encompass a high degree of variability across all parameters. This selection aimed to capture a broad representation of the DS, facilitating the training of a machine learning model, which was subsequently employed to predict the material strength of the remaining 43,917 formulations.

3) The model predictions are instrumental in ranking the formulations according to the predicted strength. However, the selection of candidates was also informed by strategic criteria. In the first three cycles (exploration phase), prediction uncertainty was given double weight in the candidate ranking. Given the relatively high prediction error at this stage, samples with higher uncertainties are deemed more valuable for enhancing the model's learning capabilities. In the subsequent two cycles (explore and exploit phase), the weight of uncertainty in sample selection was reduced to one, balancing the focus between exploring uncertain designs and exploiting predictions. In the final cycle (exploitation phase) solely the predictive capabilities of the model were exploited to select optimal formulations. The selection process also considered the novelty of each mix. This criterion, provided by SLAMD, assessed how different the parameter configuration was from previously tested materials, with novel designs potentially offering broader insights into the DS. Lastly, the intuition of lab personnel played a crucial role in the selection process in cases of uncertainty, ensuring that the selection of meaningful designs was both informed and strategic.

A detailed description of the material design process with SLAMD can be found in Völker et al [17].

3.2. Experimental Procedure for Design of Experiments with Minitab

In contrast, the Design of Experiments (DOE) plans the experimental investigation to efficiently understand the influence of various factors, such as the amount and composition of the activator solution, on the material properties.

1) Initially a design plan had to be selected. The Box-Behnken design is particularly suitable because it strategically excludes vertices that are more likely to express workability problems. Moreover, it can determine quadratic relationships between factors, allowing for nuanced analysis of nonlinear interactions. Three factor levels were chosen to limit the number of experimental runs, the minimum and maximum as shown in Table 2 plus a 50% level.

2) The design of experiment software generated an experimental plan based on the specified input, which included 46 mixtures to be tested.

3) After testing all 46 mixtures the model was generated and based on the regression formula determined, an optimized mixture was found and prepared. The model is accompanied by a comprehensive statistical analysis of the factors and the goodness of prediction, and provides several insights into the design space and the factor relationships.

4. RESULTS

The results of the experimental runs are shown in terms of the compressive strength achieved for each day in the laboratory. Figure 1 shows the DDD run results for each design phase. There is exactly one week between each laboratory day to allow the 7-day strength test data to be used as feedback for the DDD sample selection. In total, 34 geopolymer designs were validated, representing 612 laboratory strength tests.

In Figure 1, the results of the DOE-based design approach are shown on the left side. Compared to DDD the training phase is exhaustive and only the final formulation is derived from the DOE model analysis. The average performance achieved by the DDD is 89 MPa. However, the laboratory results clearly show a progressive average increase in strength over the course of the design stages (see Table A-1 in the Appendix). The highest compressive strength was achieved in the last cycle (125.5 MPa), and 12 samples reached the 100 MPa target.

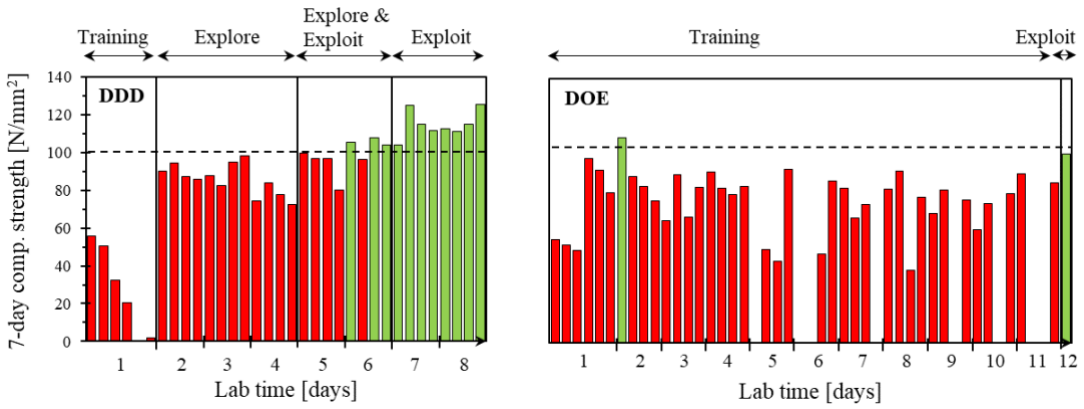

Figure 1: The 7-day compressive strength results from the data-driven design and the design of experiments approach with the goal of achieving 100 N/mm^2. The respective design phases are indicated by the arrows above.

The DOE approach led to the preparation and testing of 47 geopolymer mixtures, equivalent to 846 strength tests. The average performance of DOE designs was comparatively lower than with the DDD, at 61 MPa, and including 8 designs that failed to develop any strength. Only one mixture achieved a compressive strength above the 100 MPa mark during the training phase (108.7 MPa). The optimized mixture predicted by the DOE model reached the targeted strength, by a close margin, achieving 100.2 MPa.

The targeted progression of the data-driven experiment toward higher performing samples

becomes evident in Figure 2, A which illustrates the design space. An irregular design space was explored, and it is clear that in later stages of the experiment, high-performance materials were found in the green region.

Conversely, the design space explored by DOE (Figure 2, B) is strictly regular in its dimensions and with respect to the sample compositions studied, except for the optimized mixture shown in green with an "x". However, the highest strength was obtained during the model building phase, highlighted by the star.

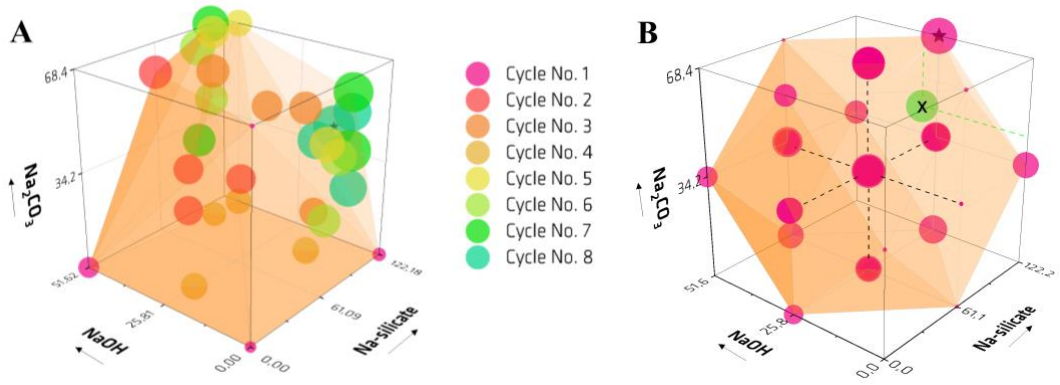

Figure 2: Lower dimensional representation of design spaces that were explored by DDD (A) and DOE (B). The size of the points reflects the compressive strength reached after 7 days. The highest strength is marked with a star. The optimized mixture from DOE is marked with an X. The variation of the W/S ratio and the sodium sulphate content are not shown.

5. CONCLUSION

This study embarked on a comparative analysis of two prevalent materials design methodologies, Design of Experiments (DOE) and Data-Driven Design (DDD), within a laboratory setting to address the inherent challenges posed by the high complexity and variability of secondary resources in materials design. The investigation delineated the processes and fundamental differences between the two approaches, with DOE aiming to representatively model the design space and DDD focusing on iterative navigation toward performance goals.

We postulated that the application of DDD methodologies can substantially accelerate the experimental development process for complex materials design, which was clearly confirmed by our comparative analysis of DDD and DOE. In particular, the investigation of the first research question yielded a compelling answer: both, the DOE and AI methodologies, as represented by DDD, contribute significantly to the mix design process for alkali-activated materials, albeit in significantly different capacities. DDD demonstrated a faster and more efficient route to high-performance material formulations, supporting our hypothesis with a

clear preference for the DDD approach in terms of speed, efficiency, and adaptability.

DDD not only accelerated the design process but also resulted in a higher quality of final mix designs, as evidenced by the success rate (33% and 4% for DDD and DOE, respectively) and the performance of the developed materials. The comparative analysis highlighted the limitations of DOE, particularly the need for a lengthy training phase within a predetermined experimental design, which may include numerous unfavorable mix designs and a comparatively weak final model.

ACKNOWLEDGMENTS

This study is supported by Bundesministerium für Bildung und Forschung by the Project PHöMixBeton (grant number 01LJ2006C) and the European Union under NextGenerationEU. Moreover, we gratefully acknowledge support from the European Union's Horizon Europe research and innovation program under grant agreement No. 101056773 for funding this work under the Reincarnate project.

REFERENCES

[1] Provis, J. L., & van Deventer, J. (2014). Alkali Activated Materials, State-of-the-Art Report, *RILEM TC 224-AAM*. *Springer*.

[2] Nikravan, M., et al. (2023). Life cycle assessment of alkali-activated materials: a systematic literature review. *Low carbon materials and green construction*, 1(13).

[3] Snellings, R., Suraneni, P., & Skibsted, J. (2023). Future and emerging supplementary cementitious materials. *Cement and concrete research*, 171(107199).

[4] Firdous, R., et al. (2021). Reaction of calcium carbonate minerals in sodium silicate solution and its role in alkali-activated systems. *Minerals Engineering*, 165(106849).

[5] Firdous, R., & Stephan, D. (2020). Impact of the mineralogical composition of natural pozzolan on properties of resultant geopolymers. *Journal of sustainable cement-based materials*, 10(3), 149-164.

[6] Firdous, R., et al. (2022). Assessment of environmental, economic and technical performance of geopolymer concrete: a case study. *Journal of Materials Science*, 57, 18711-18725.

[7] Naderpour, H., et al. (2018). Compressive strength prediction of environmentally friendly concrete using artificial neural networks. *Journal of Building Engineering*, 16, 213-219.

[8] Ben, C. W., Flah, M., & Nehdi, M. (2020). Machine learning prediction of mechanical properties of concrete: Critical review. *Construction and Building Materials*, 260.

[9] Li, Y., Lin, H., Shen, J., & Li, Y. (2023). Optimization design for alkali-activated slag-fly ash geopolymer concrete based on artificial intelligence considering compressive strength, cost, and carbon emission. *Journal of Building Engineering*, 75.

[10] Li, Z., Yoon, J., & Zhang, R. et al. (2022). Machine learning in concrete science: applications, challenges, and best practices. *Npj Computational Materials*, 8(6), p. 127.

[11] Ling, J., et al. (2017). High-Dimensional Materials and Process Optimization Using Data-Driven Experimental Design with Well-Calibrated Uncertainty Estimates. *Integrating Materials and Manufacturing Innovation*, 207-217.

[12] Golafshani, E., & Behnood, A. (2021). Predicting the mechanical properties of sustainable concrete containing waste foundry sand using multi-objective ANN approach. *Construction and Building Materials*, 291, 123314.

[13] Zhang, J., et al. (2021). Mixture optimization for environmental, economical and mechanical objectives in silica fume concrete: A novel framework based on machine learning and a new meta-heuristic algorithm. *Resources, Conservation and Recycling*, 167, 105395.

[14] Shobeiri, V., et al. (2022). A generic framework for augmented concrete mix design: Optimization of geopolymer concrete considering environmental, financial and mechanical properties. *Journal of Cleaner Production*, 369, 133382.

[15] Völker, C., Firdous, R., Stephan, D., & Kruschwitz, S. (2021). Sequential learning to accelerate discovery of alkali-activated binders. *Journal of Materials Science*, 15859-15881.

[16] Völker, C., et al. (2023). Data driven design of Alkali-activated concrete using Sequential Learning. *Journal of Cleaner Production*, 1-40.

[17] Völker C, Torres B. M., Zia G. A., Firdous R., Rug T., et al. 2023. *Presenting SLAMD – A Sequential Learning Based Software for the Inverse Design of Sustainable Cementitious Materials*. *NanoWorld Journal*, 9(S2), 180-S187.

APPENDIX

Table A-1: Detailed results from DDD

1st Dev. Cycle

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation		
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa
T-1	500	51.62	0	0	0	0.5	39	56	66	3	4	3
T-2	500	51.62	0	0	0	0.55	33	51	63	2	3	4
T-3	500	0	122.18	0	0	0.55	0	33	53	0	1	1
T-4	500	0	0	91.72	0	0.55	0	20	35	0	4	3
T-5	500	0	0	0	68.4	0.55	0	0	0	0	0	0
T-6	500	0	122.18	0	0	0.6	0	2	40	0	0	3
							Average:	27				

2nd Dev. Cycle

Curiosity 2

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
1	400	46.46	73.31	9.17	6.84	0.5	63	90	104	1	3	1	56
2	400	41.3	110	82.55	13.7	0.5	74	94	110	5	8	7	56
3	400	41.3	61.1	91.72	27.36	0.5	62	87	101	3	2	5	56
4	400	36.13	24.44	27.52	68.4	0.5	61	86	88	1	4	4	56
							Average:	89				Average:	56
												ø Error:	**33**

3rd Dev. Cycle

Curiosity 2

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
5	400	20.65	122.18	18.34	6.84	0.6	62	88	91	2	3	2	64
6	400	20.65	73.31	18.34	54.72	0.6	58	82	86	2	6	3	62
7	400	20.65	109.96	18.34	47.88	0.55	64	95	104	5	5	4	65
8	400	46.46	97.74	0	54.72	0.5	73	100	111	4	5	8	66
							Average:	91				Average:	64
												ø Error:	**27**

4th Dev. Cycle

Curiosity 2

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
9	400	46.46	97.74	0	0	0.6	47	74	93	1	4	5	77
10	400	46.46	122.18	64.2	0	0.6	62	84	101	2	4	5	75
11	400	15.49	97.74	9.17	0	0.5	53	78	96	2	4	3	78
12	400	25.81	24.44	91.72	0	0.55	46	72	78	2	3	2	68
							Average:	77				Average:	75
												ø Error:	**2**

5th Dev. Cycle

Curiosity 1

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
13	400	10.32	97.74	9.172	41.04	0.5	64	100	106	4	6	7	73
14	400	46.46	97.74	9.172	68.4	0.5	71	97	106	2	3	5	89
15	400	10.32	97.74	45.86	41.04	0.55	53	95	101	1	3	6	72
16	400	46.46	122.18	45.86	68.4	0.55	60	80	95	5	5	4	87
							Average:	93				Average:	80
												ø Error:	**13**

6th Dev. Cycle

Curiosity 1

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
17	400	10.32	110.0	18.34	34.20	0.5	63	106	110	3	4	6	90
18	400	10.32	97.74	45.86	13.68	0.5	60	96	94	2	2	6	89
19	400	51.62	97.74	0.00	61.56	0.5	74	107	109	4	8	4	92
20	400	51.62	110.0	9.17	41.04	0.5	71	104	117	4	6	11	92
							Average:	104				Average:	91
												ø Error:	**13**

7th Dev. Cycle

Curiosity 1 resp. 0

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
21	400	51.62	97.74	64.20	27.36	0.5	73	104	124	2	4	7	99
22	400	10.32	122.2	0.00	34.20	0.5	70	125	123	3	6	6	101
23	400	10.32	122.2	18.34	54.72	0.5	68	115	127	3	4	9	100
24	400	51.62	110.0	0.00	68.40	0.5	80	111	109	2	3	5	103
							Average:	114				Average:	100
												ø Error:	**13**

8th Dev. Cycle

Curiosity 0

Model Random Forest

IDX	Powder	Salt				w/s	Compressive Strength			Standard Deviation			Prediction
		NaOH	Na-silicate	Na2SO4	Na2CO3		1-day	7-days	28-days	1 day	7-days	28-days	7-days
	g	g	g	g	g		MPa	MPa	MPa	MPa	MPa	MPa	MPa
25	400	10.32	122.2	0.00	20.52	0.5	79	112	112	3	6	4	114
26	400	10.32	122.2	0.00	47.88	0.5	81	111	113	4	6	7	114
27	400	20.65	122.2	0.00	34.20	0.5	84	115	117	5	7	7	113
28	400	15.49	122.2	0.00	41.04	0.5	82	126	124	4	3	4	114
							Average:	116				Average:	114
												ø Error:	**2**

Table A-2: Detailed results from DOE, including the 1, 7 and 28-day compressive strength.

	Activator Compounds [g]					Compressive Strength [MPa]			Standard Dev. [MPa]		
Nr.	**Na-Silicate**	**Na_2SO_4**	**Na_2CO_3**	**NaOH**	**W/S**	**1d**	**7d**	**28d**	**1d**	**7d**	**28d**
1	0.00	45.85	34.20	51.60	0.55	52.3	54.7	66.7	3.9	8.4	4.3
2	0.00	45.85	68.40	25.80	0.55	13.0	51.9	47.4	1.6	5.3	14.5
3	0.00	45.85	0.00	25.80	0.55	37.4	49.1	53.0	4.1	3.2	18.7
4	61.10	45.85	34.20	25.80	0.55	57.9	97.6	85.4	4.4	3.4	12.7
5	122.20	91.70	34.20	25.80	0.55	71.5	91.5	118.0	5.3	12.5	17.3
6	122.20	45.85	34.20	25.80	0.50	53.0	79.4	94.0	2.0	9.6	9.8
7	122.20	45.85	68.40	25.80	0.55	67.1	108.6	110.0	4.0	6.7	24.3
8	61.10	0.00	34.20	25.80	0.50	59.6	87.9	98.4	5.8	3.0	6.1
9	61.10	45.85	34.20	25.80	0.55	66.4	82.8	73.1	5.7	6.4	9.4
10	61.10	45.85	34.20	51.60	0.60	58.3	75.5	93.7	3.0	10.3	6.3
11	0.00	45.85	34.20	25.80	0.60	32.2	64.6	59.2	1.7	4.6	7.6
12	61.10	0.00	68.40	25.80	0.55	64.4	89.0	76.7	1.3	3.7	2.7
13	0.00	45.85	34.20	25.80	0.50	40.1	66.6	72.2	2.8	8.0	12.0
14	61.10	45.85	34.20	25.80	0.55	55.6	71.3	100.6	3.7	9.5	9.6
15	61.10	0.00	34.20	51.60	0.55	58.5	74.9	83.1	9.7	8.3	12.8
16	61.10	91.70	68.40	25.80	0.55	57.2	81.9	89.5	5.4	8.5	10.0
17	61.10	45.85	68.40	25.80	0.60	51.9	78.6	87.7	4.7	7.1	12.1
18	122.20	45.85	34.20	25.80	0.60	53.6	82.9	82.8	10.0	11.1	13.4
19	61.10	45.85	0.00	0.00	0.55	0.0	0.0	10.7	0.0	0.0	1.4
20	61.10	0.00	34.20	25.80	0.60	27.5	59.3	64.6	6.6	2.3	6.2
21	0.00	91.70	34.20	25.80	0.55	33.4	50.1	59.3	3.8	4.4	4.3
22	61.10	45.85	34.20	51.60	0.50	66.2	91.8	84.5	2.5	2.6	15.7
23	61.10	45.85	34.20	0.00	0.50	0.0	0.0	56.5	0.0	0.0	13.4
24	61.10	45.85	34.20	0.00	0.60	0.0	0.0	0.0	0.0	0.0	0.0

	Activator Compounds [g]					Compressive Strength [MPa]			Standard Dev. [MPa]		
Nr.	**Na-Silicate**	**Na_2SO_4**	**Na_2CO_3**	**NaOH**	**W/S**	**1d**	**7d**	**28d**	**1d**	**7d**	**28d**
25	0.00	0.00	34.20	25.80	0.55	33.3	47.2	62.7	2.2	5.7	2.1
26	61.10	45.85	34.20	25.80	0.55	53.1	85.8	84.0	9.4	5.5	4.2
27	61.10	45.85	0.00	51.60	0.55	58.0	81.9	89.9	7.0	7.5	12.0
28	61.10	91.70	34.20	51.60	0.55	56.4	66.2	92.0	9.4	13.9	12.5
29	122.20	45.85	34.20	0.00	0.55	24.7	73.2	82.0	15.8	11.7	10.0
30	61.10	0.00	34.20	0.00	0.55	0.0	0.0	0.0	0.0	0.0	0.0
31	61.10	45.85	34.20	25.80	0.55	53.5	81.5	94.3	7.7	6.3	5.4
32	122.20	45.85	0.00	25.80	0.55	58.1	91.0	106.5	3.4	10.8	3.6
33	61.10	0.00	0.00	25.80	0.55	10.4	38.5	55.6	10.0	7.0	4.6
34	61.10	45.85	0.00	25.80	0.50	58.3	77.3	90.1	2.6	3.4	6.0
35	61.10	91.70	0.00	25.80	0.55	43.8	68.6	80.5	10.1	10.7	15.4
36	61.10	45.85	34.20	25.80	0.55	46.2	81.1	98.6	17.3	11.5	6.4
37	61.10	45.85	68.40	0.00	0.55	0.0	0.0	0.0	0.0	0.0	0.0
38	61.10	91.70	34.20	25.80	0.50	55.0	75.8	93.6	5.3	12.2	11.2
39	61.10	45.85	0.00	25.80	0.60	34.2	59.9	77.6	3.6	13.4	14.9
40	122.20	45.85	34.20	51.60	0.55	65.4	73.8	91.3	11.0	5.1	13.9
41	61.10	91.70	34.20	0.00	0.55	0.0	0.0	0.0	0.0	0.0	0.0
42	61.10	91.70	34.20	25.80	0.60	50.9	79.3	90.5	5.3	4.6	3.8
43	61.10	45.85	68.40	25.80	0.50	55.8	89.3	103.8	6.0	16.7	14.9
44	0.00	45.85	34.20	0.00	0.55	0.0	0.0	0.0	0.0	0.0	0.0
45	61.10	45.85	68.40	51.60	0.55	0.0	0.0	0.0	0.0	0.0	0.0
46	122.20	0.00	34.20	25.80	0.55	65.1	84.7	109.0	2.3	14.6	3.3
Opt.	122.18	22.23	43.53	30.23	0.5	70.2	100.2	106.4	8.0	6.9	12.3