Concrete mix design optimization:

Leveraging machine learning and Bayesian optimization for developing low-CO_2 and cost-efficient mixtures containing SCM

Arslan Akbar,
Zachary Blume, Farshad Rajabipour

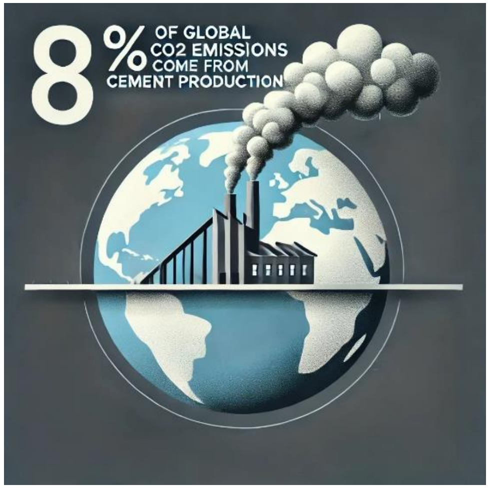
Pennsylvania State University

PennState
Institute of Energy
and the Environment

aci CONCRETE CONVENTION

Concrete emits CO_2, but alternatives are not scalable

Cement industry: a major CO_2 contributor.

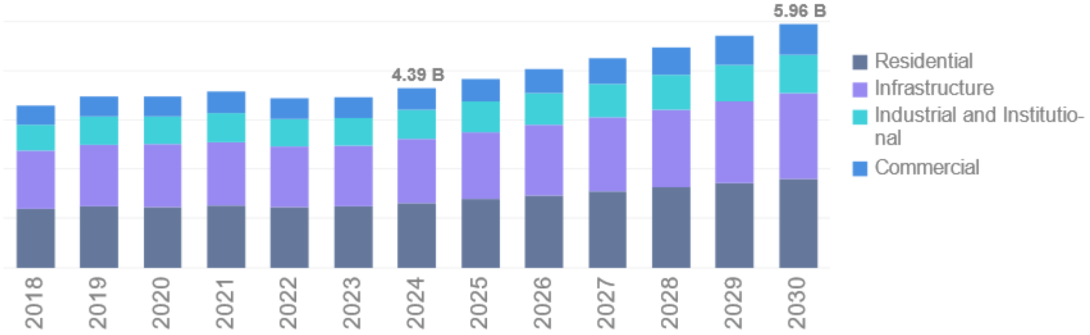


Wood a sustainable solution?

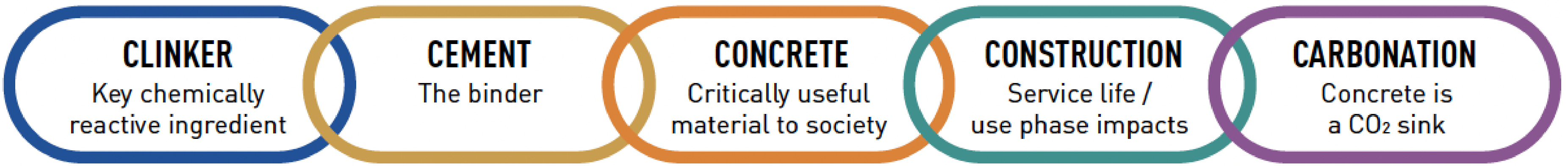
Requires new forests 1.5 times the size of India.

Source: [Energy Transition Commission]

Volume of Cement Consumed by End Use Sector, Tons, Global, 2018-2030

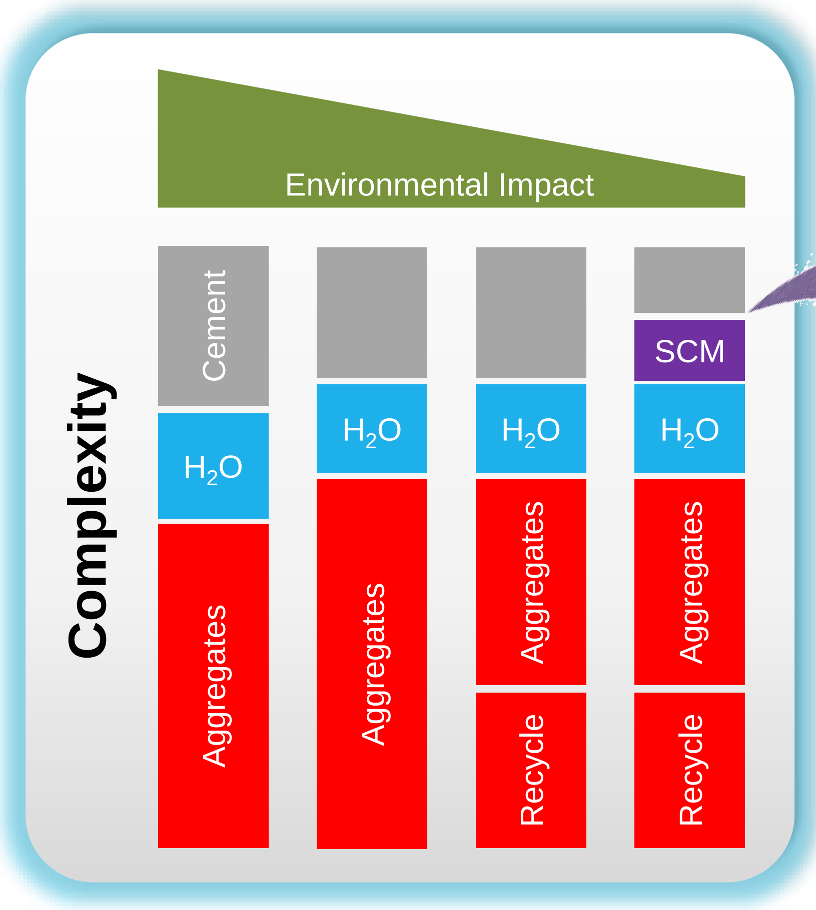


PCA roadmap to carbon neutrality

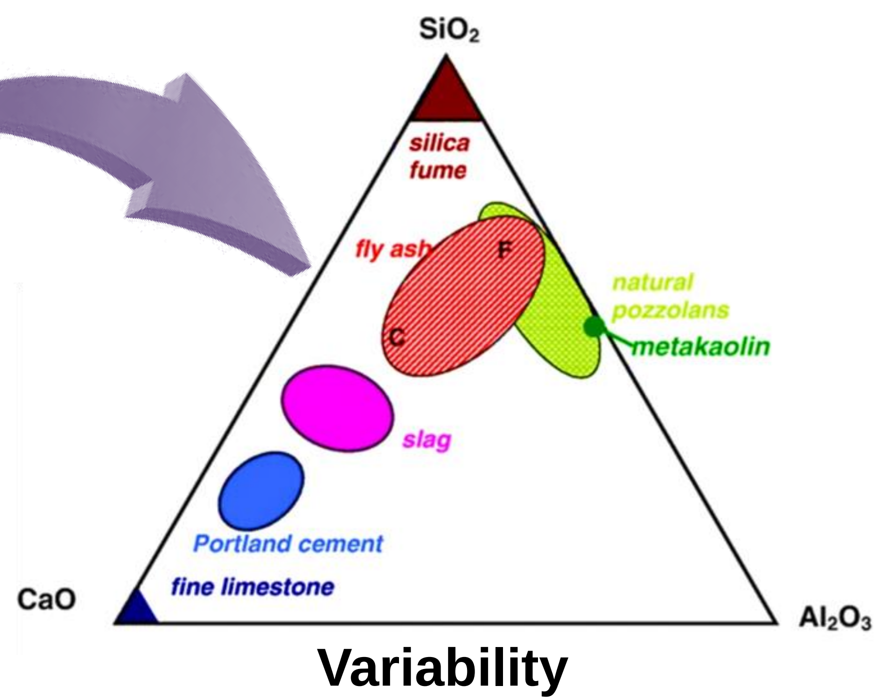


- Less CO_2 in clinker (e.g., energy efficient kilns powered by renewable electricity)
- Less clinker in cement (e.g., high SCM, geopolymers)
- Improve concrete (e.g., lean mixtures, avoid over design, recycled aggregates, seawater)
- Improve construction and maintenance (e.g., durability)
- Carbon capture and mineralization

Demand for sustainability and performance has turned concrete into a complex mixture with high SCMs and recycled materials



Need for mix design optimization to meet performance while reducing CO2/cost.



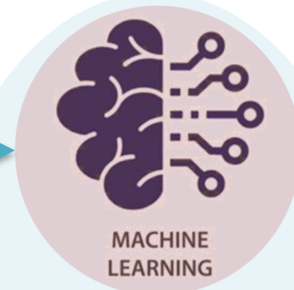
Solution: AI-assisted concrete proportioning?
Machine Learning + Bayesian Optimization

Input

Ingredients
Mix proportions

Cement, SCM, Agg properties;
w/cm, SCM/cm, Agg/cm, …

Process → Performance



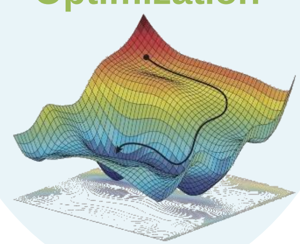
Output

Concrete Performance

Workability,
Strength,
Durability, …

Ingredients,
Concrete Performance

Mixture Optimization

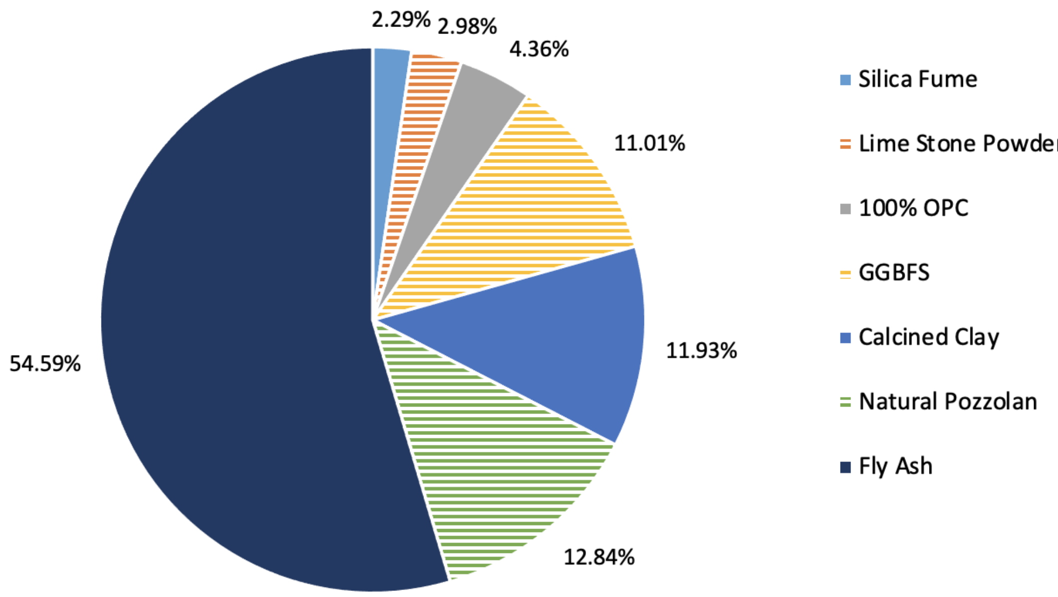


Mixture proportions

Research objectives are to develop:

1. Database:

of concrete mix designs vs strength from literature data, in-house test data, and industry contacts.

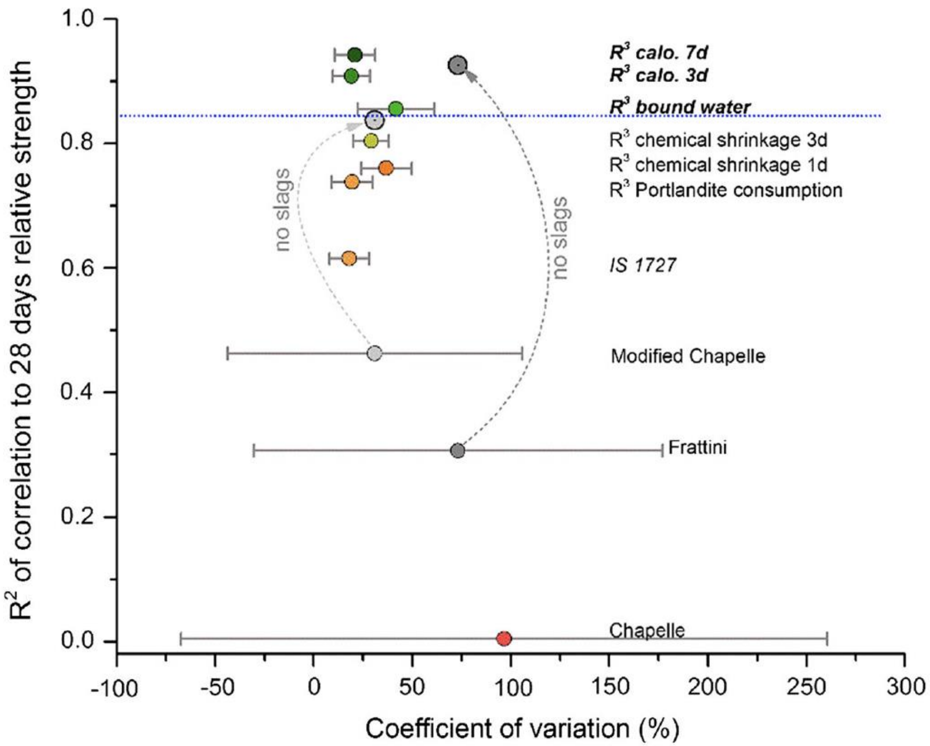


Distribution of 450 binary mix designs by SCM type in the database

Table – Example mix design input

Mix #	Cement									SCM		Mixture Proportions (By Mass)				28-Day Compressive Strength	
	CaO	SiO2	Al2O3	Fe2O3	SO3	MgO	Na2Oeq	LOI	Blaine's Fineness (m^2/kg)	Al2O3	Calorimeter R3 - 7 day (J/g)	Ratio of Bin. Cons. To (cm)			T. Agg./Bin.	$f_x(d)/f_{cy}(10)$	fu (Mpa)
												Gyp/cm	w/cm	scm/cm			
10	64.45	19.08	5.31	3.77	3.12	1.66	1.10	0.43	351	32.96	737.21	0.015	0.500	0.296	2.00	1.312	56.28

Unique model feature: Incorporating R^3 SCM Reactivity Test (ASTM C1897) that shows high correlation with concrete strength



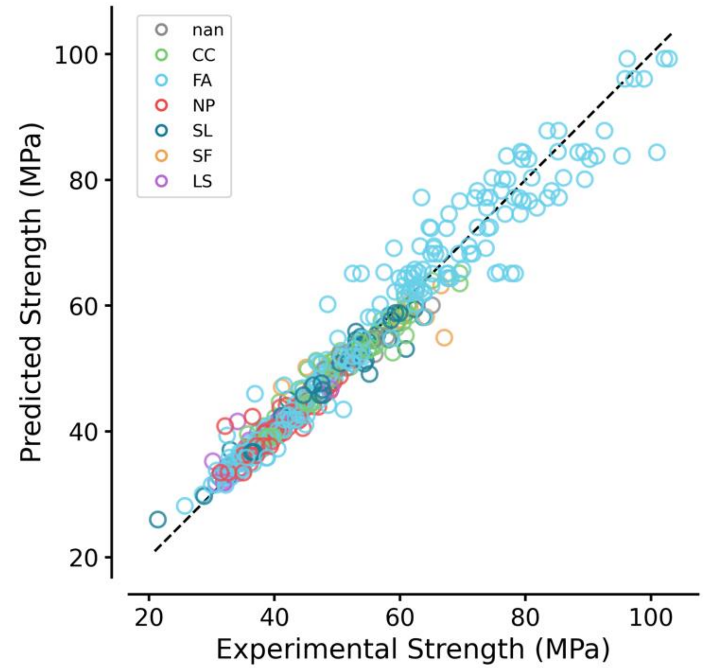
Source: Li et al. 2018

Mix design for R^3 paste, gr			
SCM	$Ca(OH)_2$	$CaCO_3$	Alkaline solution
10	30	5	54

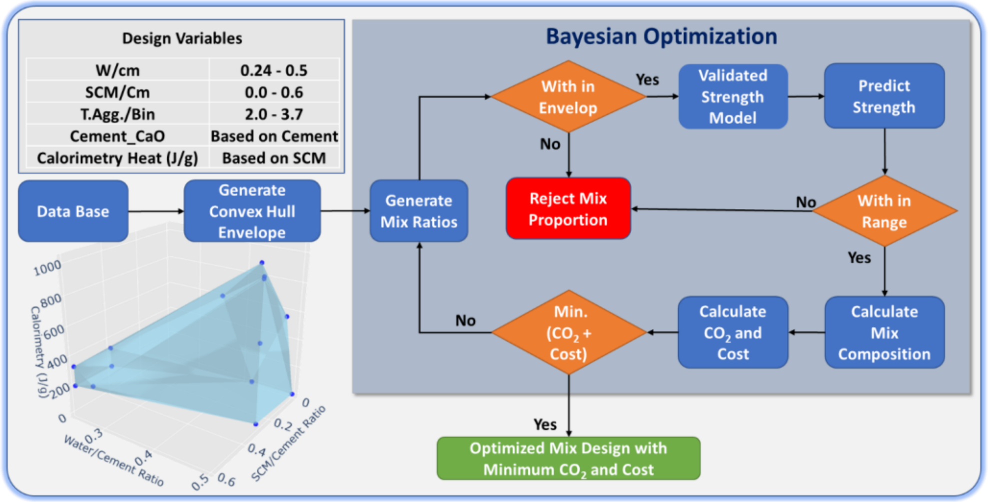
Mix for 2 mins and sealed cure at 40ºC. Measure bound water or cumulative heat of rxn at 7 days.

Research objectives are to develop:

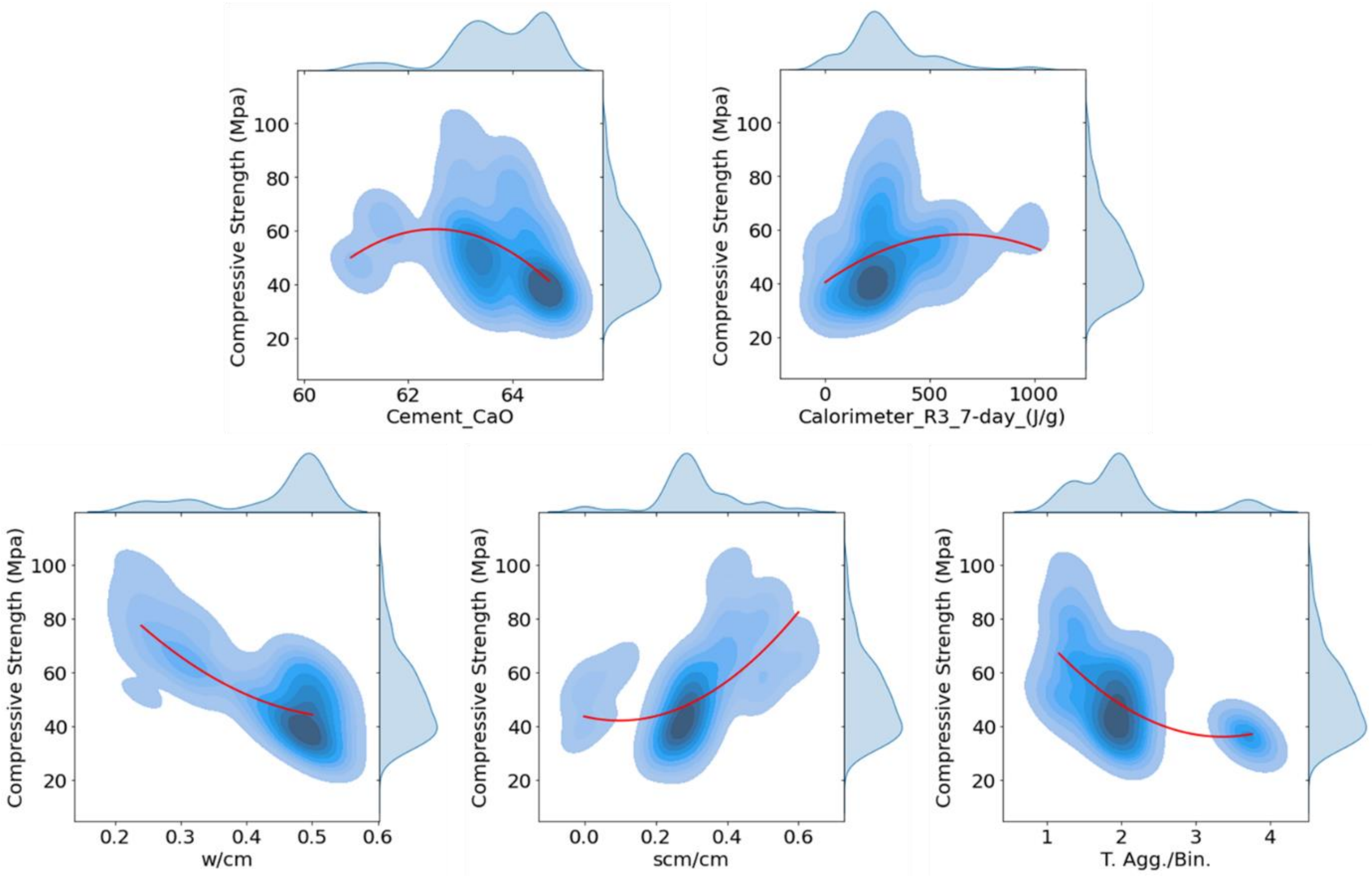
2. **Strength Model**:
   A machine learning model based on Gaussian process statistics to predict compressive strength from concrete ingredients + mix design.



3. **Mix Design Model**:
   Given available cement and SCM properties, Bayesian Optimization offers optimum mix design meeting target strength at min. CO_2 and cost



Density plots showing the distribution of input parameters and their impact on the measured strength



Feature Selection for Strength Prediction Model

Most significant strength predictors: w/cm, SCM/cm, SCM R3.

Training of the strength predictor ML model:

Random Forest Model → **Bayesian optimization for Hyper-parameter Tuning** → **10-Fold Cross Validation** → **Feature Importance Score** → **Sequential model building and evaluation**

Feature Importance score based on RF model with n number of features

↓

Incremental modeling

Set of n number of features in ascending order of their Importance Rank

↓

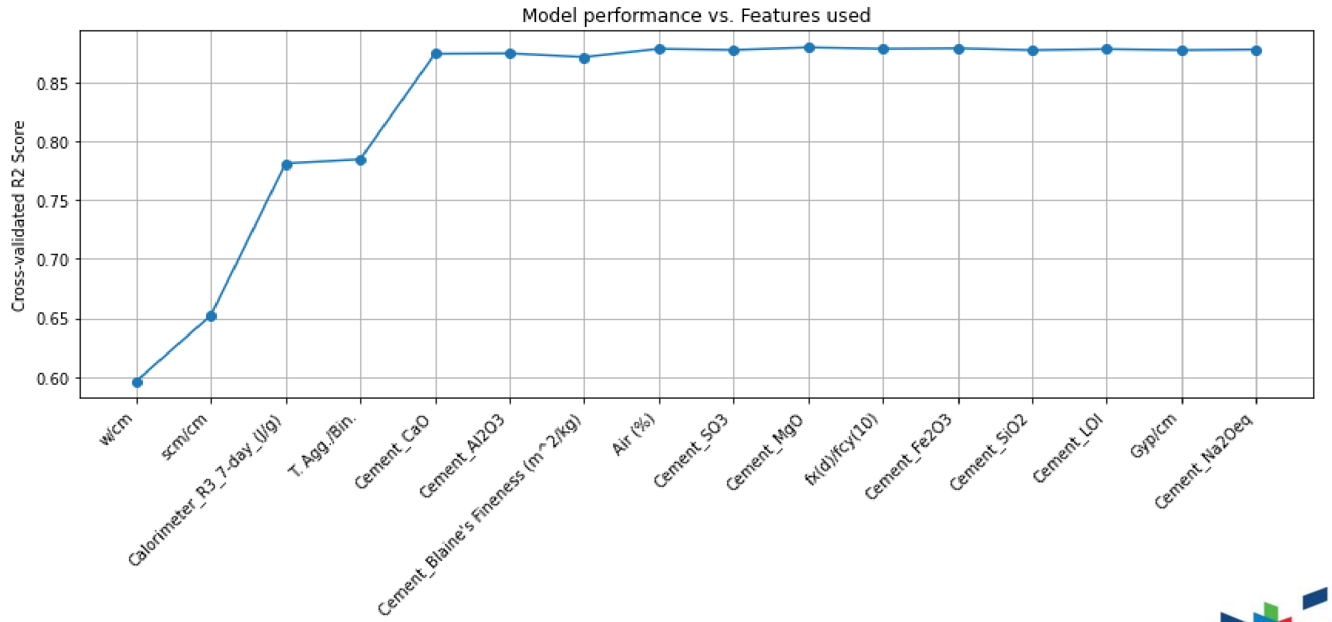
Generate subset of input features (1^{st} Ranked), (1^{st} + 2^{nd} Ranked),(1^{st} + 2^{nd} + 3^{rd} Ranked), ..., (1^{st} + 2^{nd} + ...n^{th} Ranked)

↓

Train and Validate the Models

↓

Performance Score

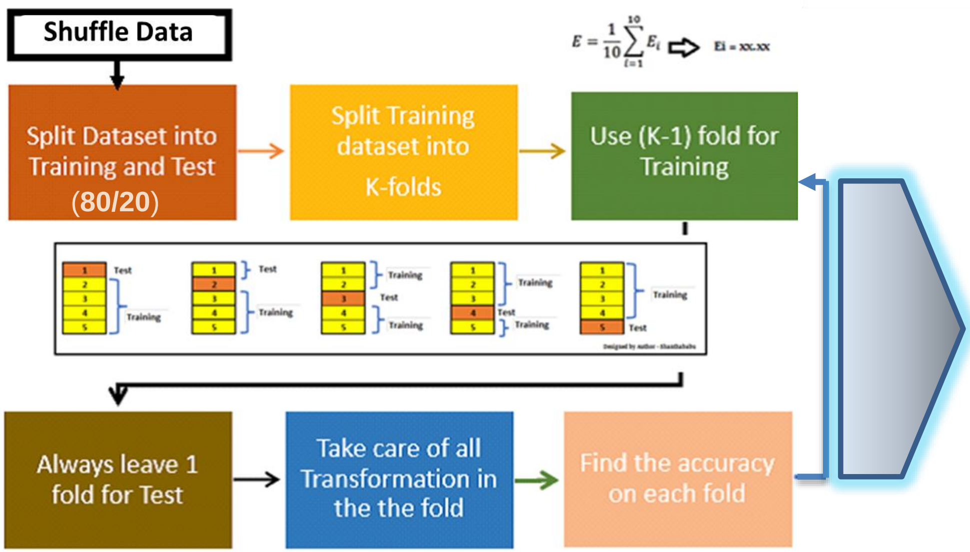


Strength model training and validation

Model Training and Validation

Optimized hyperparameters for Random Forest Prediction Model

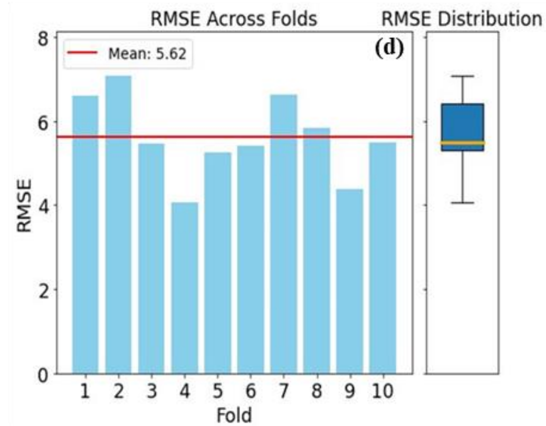
Max Depth: 15,
Max Features: 0.8,
Min samples leaf: 1.84,
Min samples split: 2,
Min weight fraction leaf: 0.002,
n estimators: 50



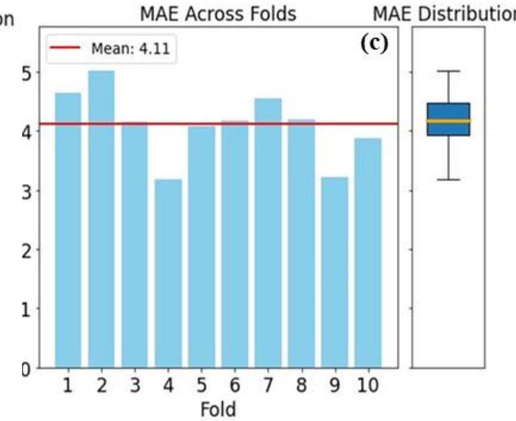
K-fold Cross Validation

Cross-Validated Error Metrics:
Mean MAE: 4.1
Mean RMSE: 5.62
Mean R^2 Score: 0.85

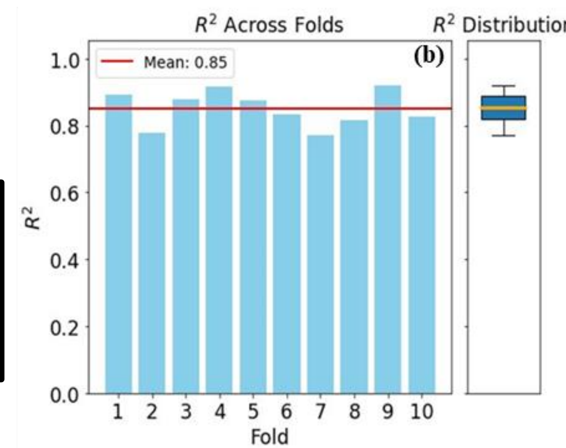
Root mean squared error



Mean absolute error



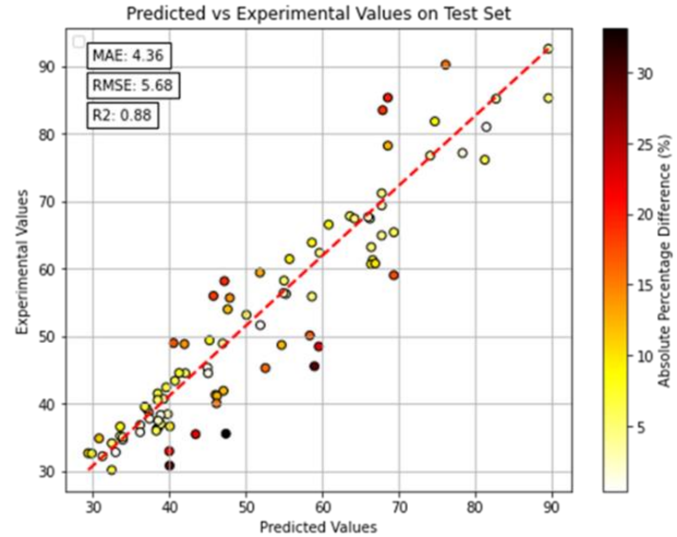
Coefficient of determination

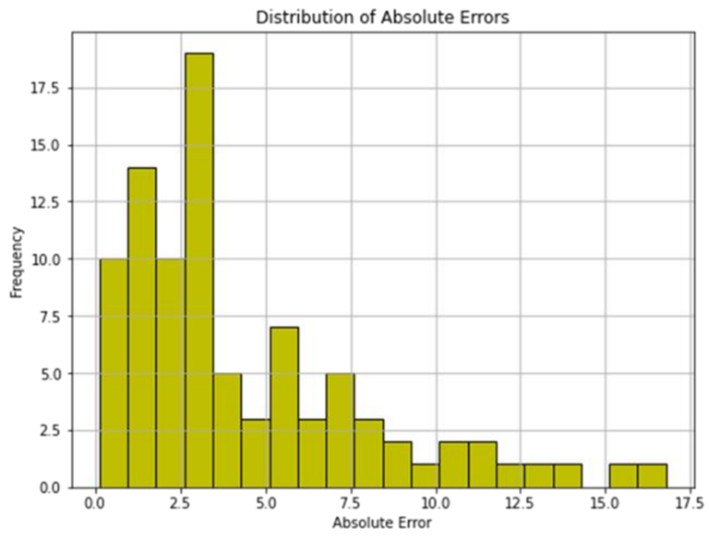


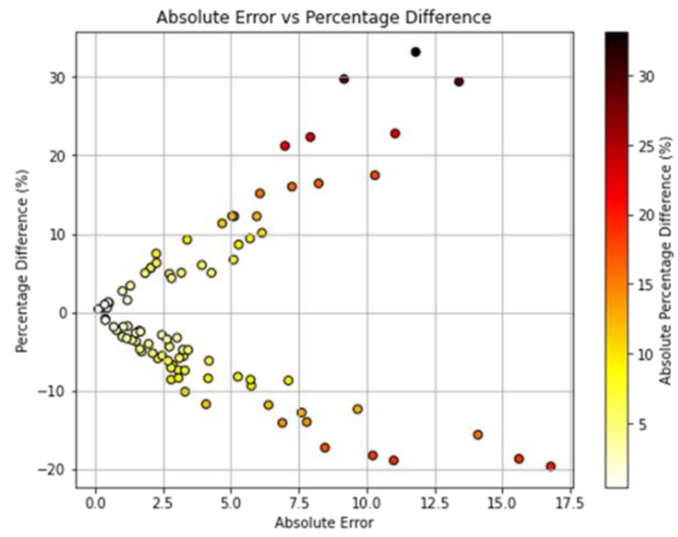
Strength model's prediction accuracy

Test the prediction accuracy of the model using 20% of data that the model was never trained on.

Final Model Evaluation:
MAE: 4.36
RMSE: 5.68
R^2 Score: 0.88







Framework for the mix design Bayesian Optimization model

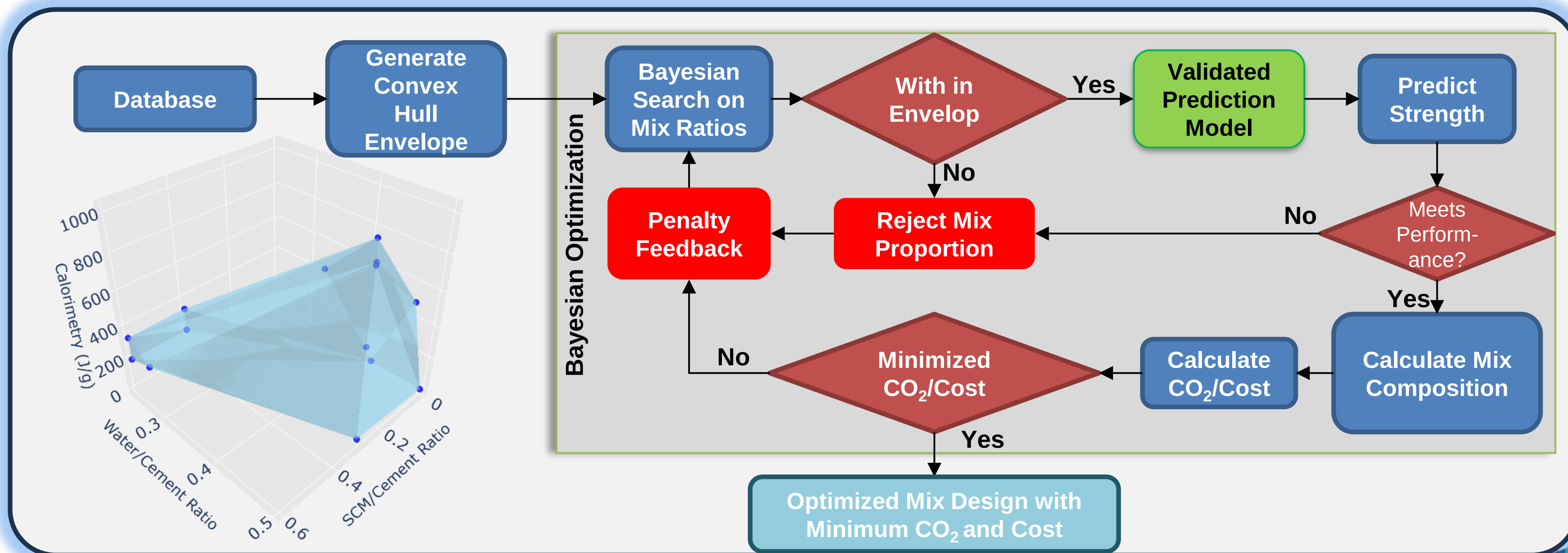
(GWP from Miller et al. 2018, cost from industry)

Material	GWP Coef. (kg CO_{2eq}/kg)	Cost ($/ton)
Cement (OPC)	0.910	130
Fly Ash (FA)	0.027	79
Slag (SL)	0.074	145
Calcined Clay (CC)	0.313	100
Natural Pozzolan (NP)	0.006	93
Limestone Filler (LS)	0.007	60
Silica Fume (SF)	0.024	650
Coarse Aggregate (CA)	0.006	21
Fine Aggregate (FA)	0.008	24
Water (W)	0.001	0
Gypsum (G)	0.008	60

Inputs:
Cement, SCM properties,
Target performance

Parameters with highest impact on strength

Design Variables	
W/cm	0.24 - 0.5
SCM/Cm	0.0 - 0.6
T.Agg./Bin	2.0 - 3.7
Cement_CaO	Based on Cement
Calorimetry Heat (J/g)	Based on SCM

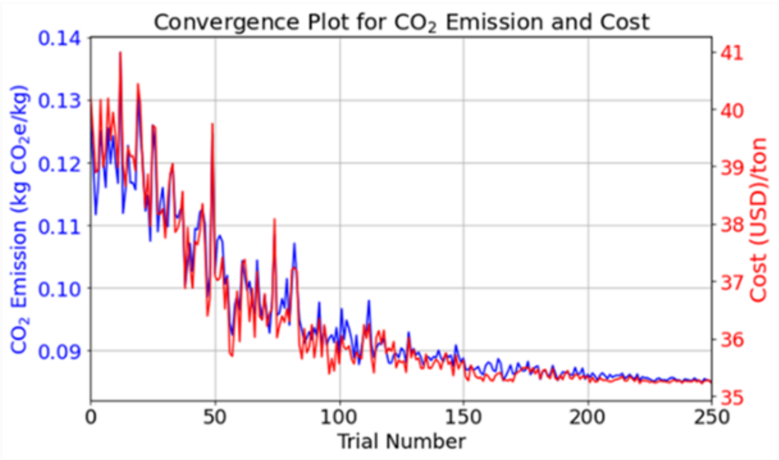


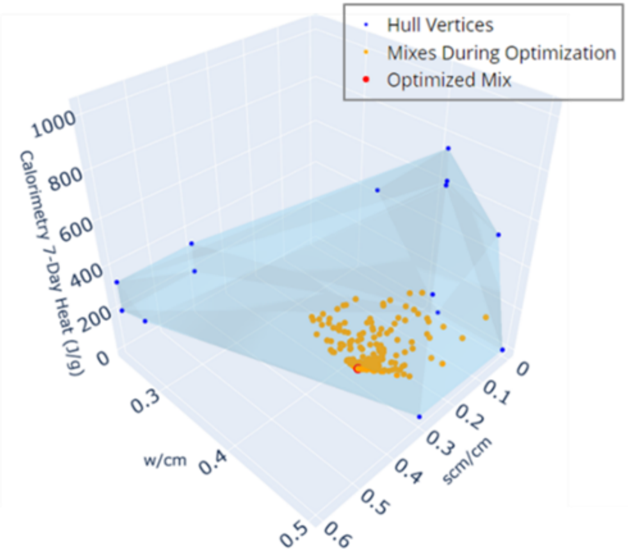
Example: optimized mix design containing fly ash for 45±5 MPa 28-day strength

Predicted strength (fu): 42.56 MPa

scm/cm: 0.37
T.Agg./Bin: 3.69
CO_2 Emission: 0.0848 kg CO_2eq/kg

w/cm: 0.45
Calorimetry Heat (J/g): 199.4
Cost: 35.213 USD/ton





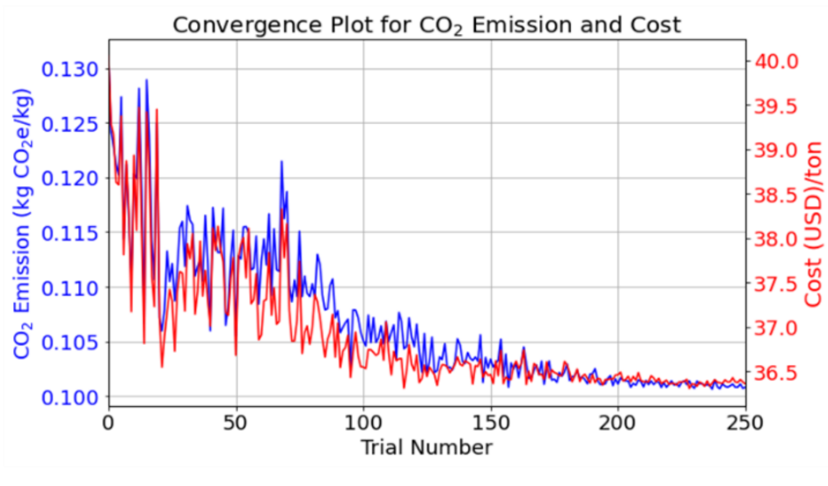
Achieves 33% CO_2 reduction and 12% cost reduction compared to first Valid Mix

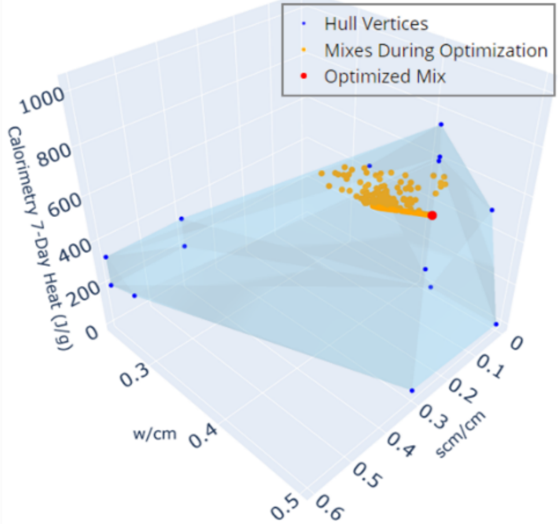
Achieves **47% CO_2 reduction compared to NRMCA** baseline concrete mix at the same 28-d f'c.

Example: optimized mix design containing calcined clay for 45±5 MPa 28-day strength

Predicted strength (fu): 47.97 MPa

scm/cm: 0.32	w/cm: 0.48
T.Agg./Bin: 3.69	Calorimetry Heat (J/g): 776.90
CO_2 Emission: 0.101 kg CO_2eq/kg	Cost: 36.18 USD/ton





Achieves 22% CO_2 reduction and 9% cost reduction compared to first Valid Mix

Achieves **37% CO_2 reduction compared to NRMCA** baseline concrete mix at the same 28-d f'c.

aci CONCRETE CONVENTION

Conclusions

- Database, Strength model, and Mix design optimization model developed.

- Strength Model predicts 28-d f'c (mean absolute error = 4.36 MPa) based on concrete mix design and properties of cement and SCM.

- Mix Design Model offers an optimum mix design of min. CO_2 and cost while meeting target strength.

- Models can be expanded to include ternary mixtures and durability performance metrics.

Thank you!

aci CONCRETE CONVENTION

Answers to Questions shared in email

- **How is this work novel and different than other ML models that exist for predicting concrete strength?**

- The novelty lies in integrating the R^3 test data, a recent ASTM standard (ASTM C1897), for SCM reactivity, and using the strength prediction model for dual optimization of low CO_2 and cost. Existing ML models, often focus on strength prediction using mix proportions, curing age, or non-destructive testing parameters like resistivity, but may not incorporate R^3 test data or optimize for environmental and cost metrics. And Most of the models do not include the variability in SCM type in concrete mixes while R3 data make this model robust to include different SCM types in one model.

Answers to Questions shared in email

- **Why is air% not considered as a high priority feature?**
- Air content has a large impact on compressive strength of concrete. However, due to limited variability of air content among mixtures available in our database, ML did not identify air content as a significant predictor of strength.

Answers to Questions shared in email

- **How to make a ML model publicly available? What kind of interface needs to be build?**
- Options include open-source code on GitHub, pre-trained model files, or web apps.