Mar 29th, 2022

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MACHINE LEARNING-BASED MIX DESIGN TOOLS TO MINIMIZE CARBON FOOTPRINT AND COST OF UHPC

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MOTIVATION OF THIS STUDY

Problem Statement

Emergence of UHPC vs Global Sustainability Efforts

- Cement production -> 8% anthropogenic CO2 emissions
- UHPC -> higher cement content per unit volume

- UHPC -> higher cost per unit volume

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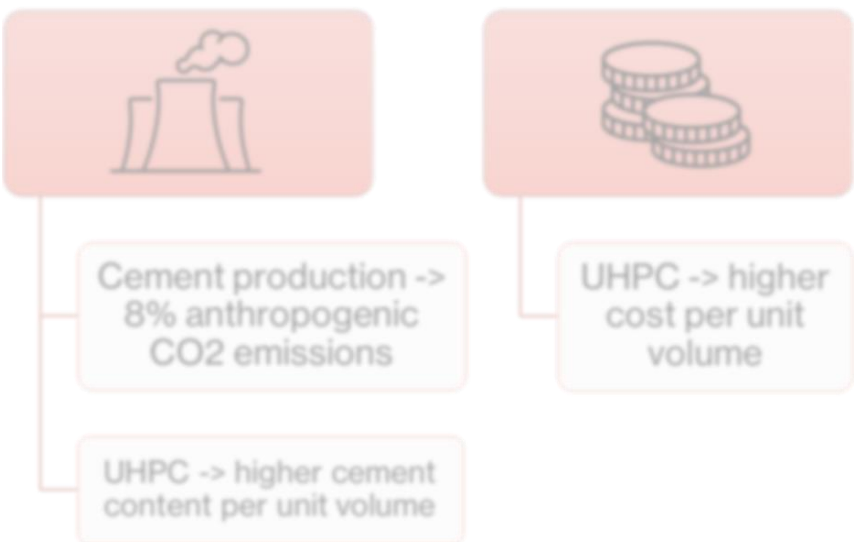

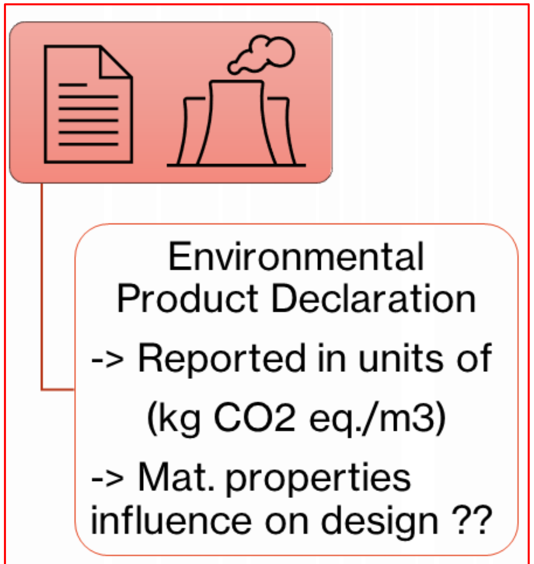

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Emergence of UHPC vs Global Sustainability Efforts

- Cement production -> 8% anthropogenic CO_2 emissions
- UHPC -> higher cement content per unit volume

- UHPC -> higher cost per unit volume

Mixture Design
-> Optimization <-

Tradeoff [performance – cost – emissions]
-> Overall visualization <-

Research Questions

Key questions addressed in this research

1. Can we accurately estimate the relationship between **compressive strength** and **mix proportions** of UHPC with a **few experimental runs & ML models**?

2. Can we evaluate the effect of changes in mix proportioning on mechanical performance in an easy and intuitive way?

3. Can we evaluate the effect of mix proportioning & mechanical performance on cost and eco-efficiency concurrently?

4. Are high paste content, high strength (and ultra-high strength) concrete technologies detrimental to cost and/or eco efficiencies?

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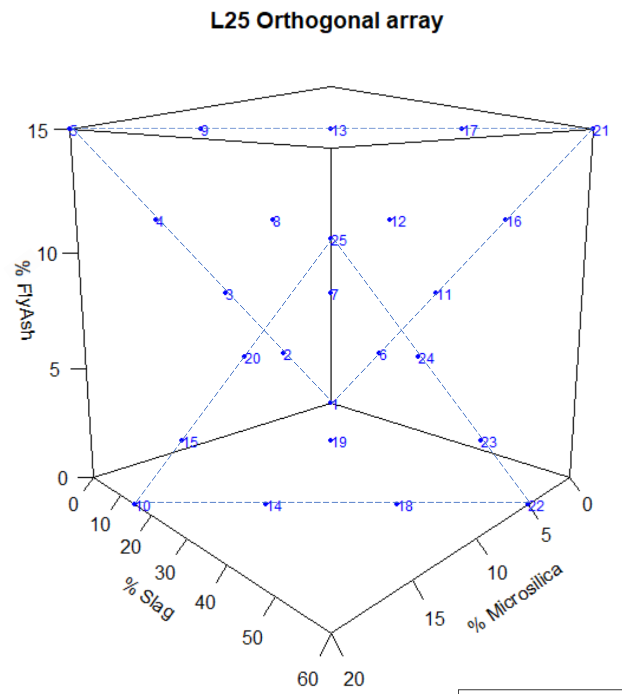
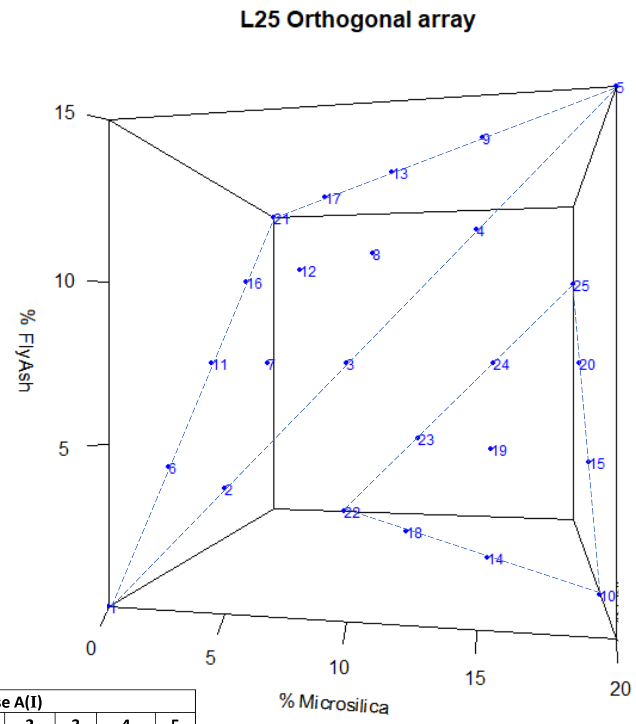
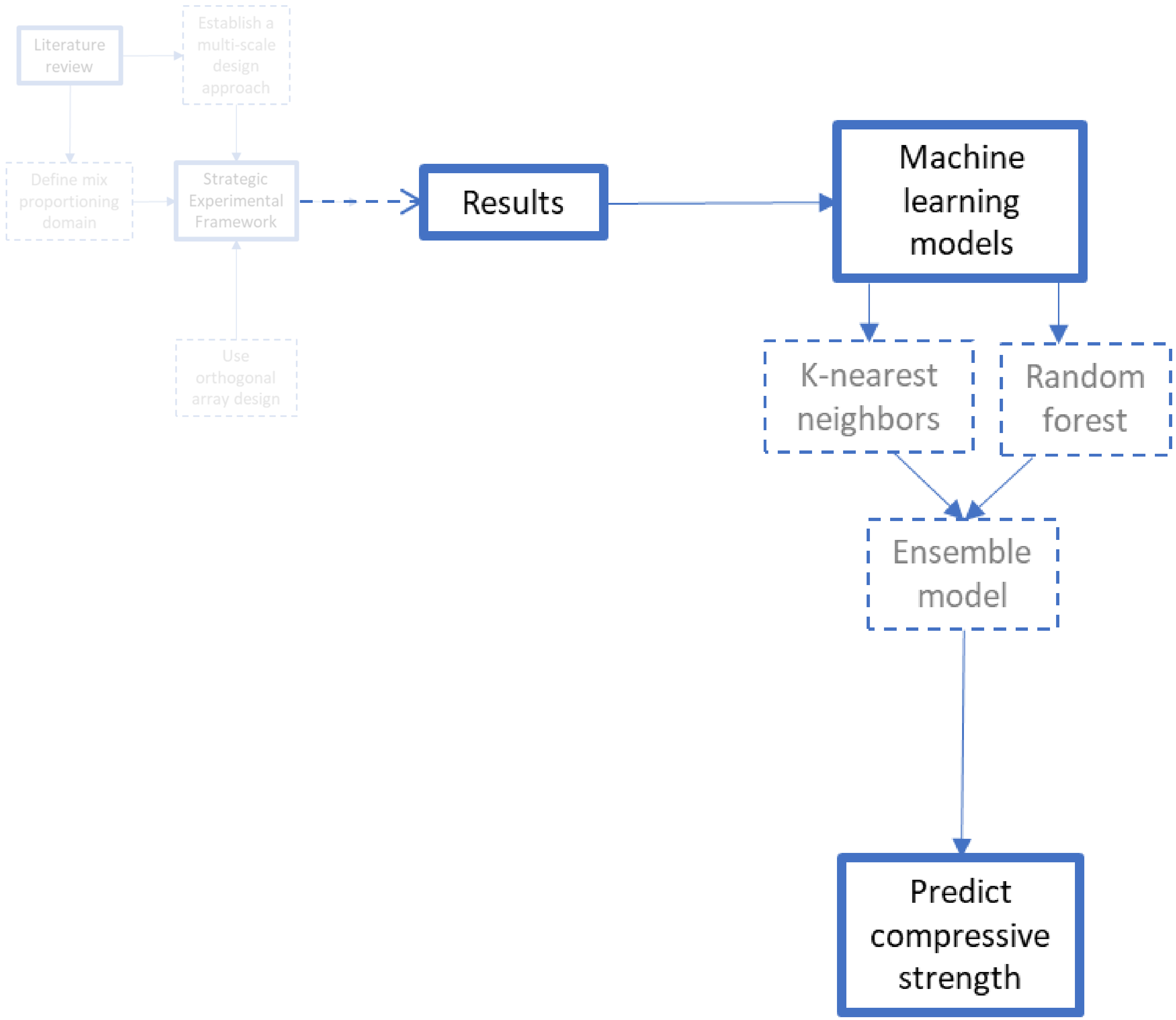
Conceptual Framework

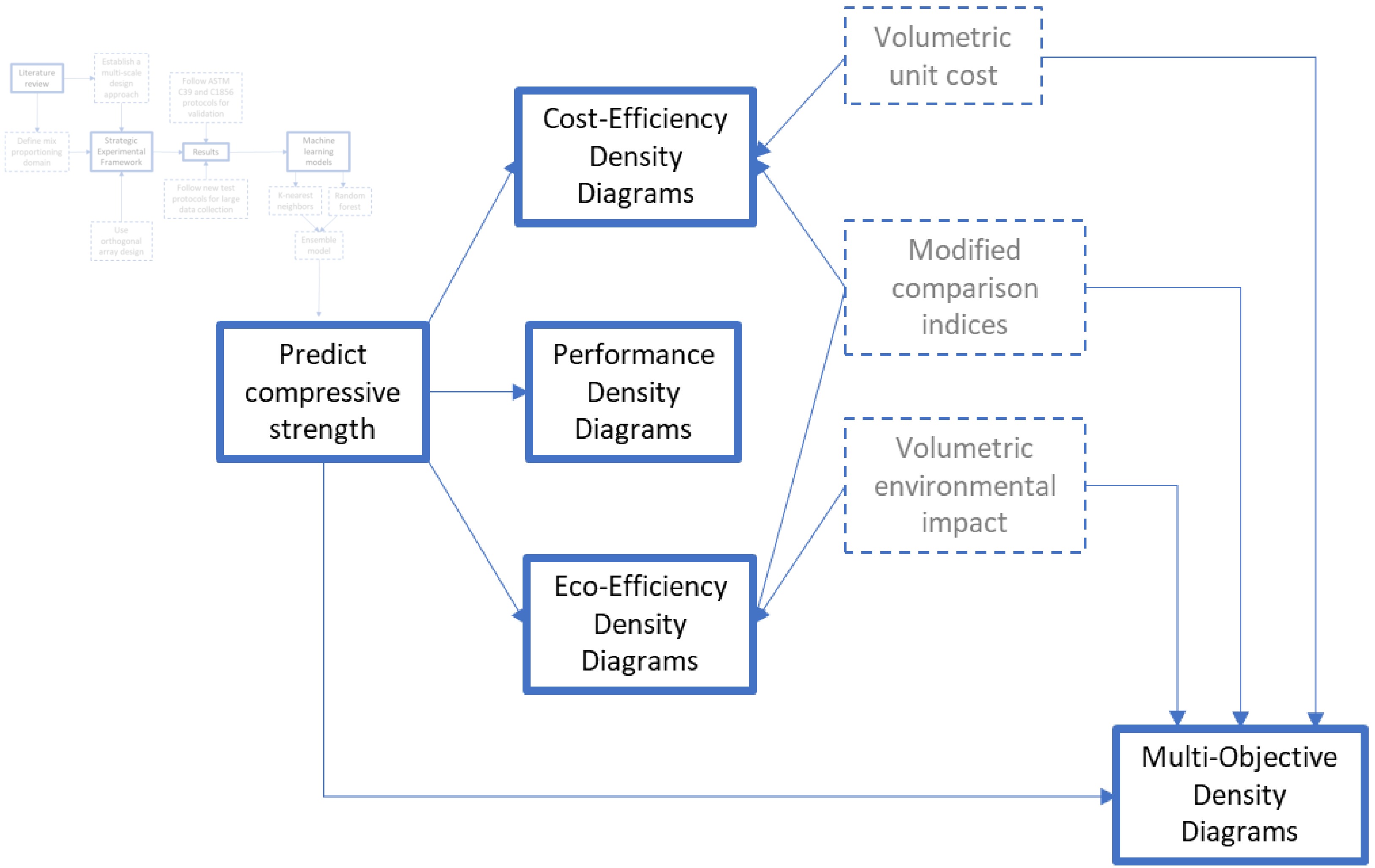
Reduced experimental runs

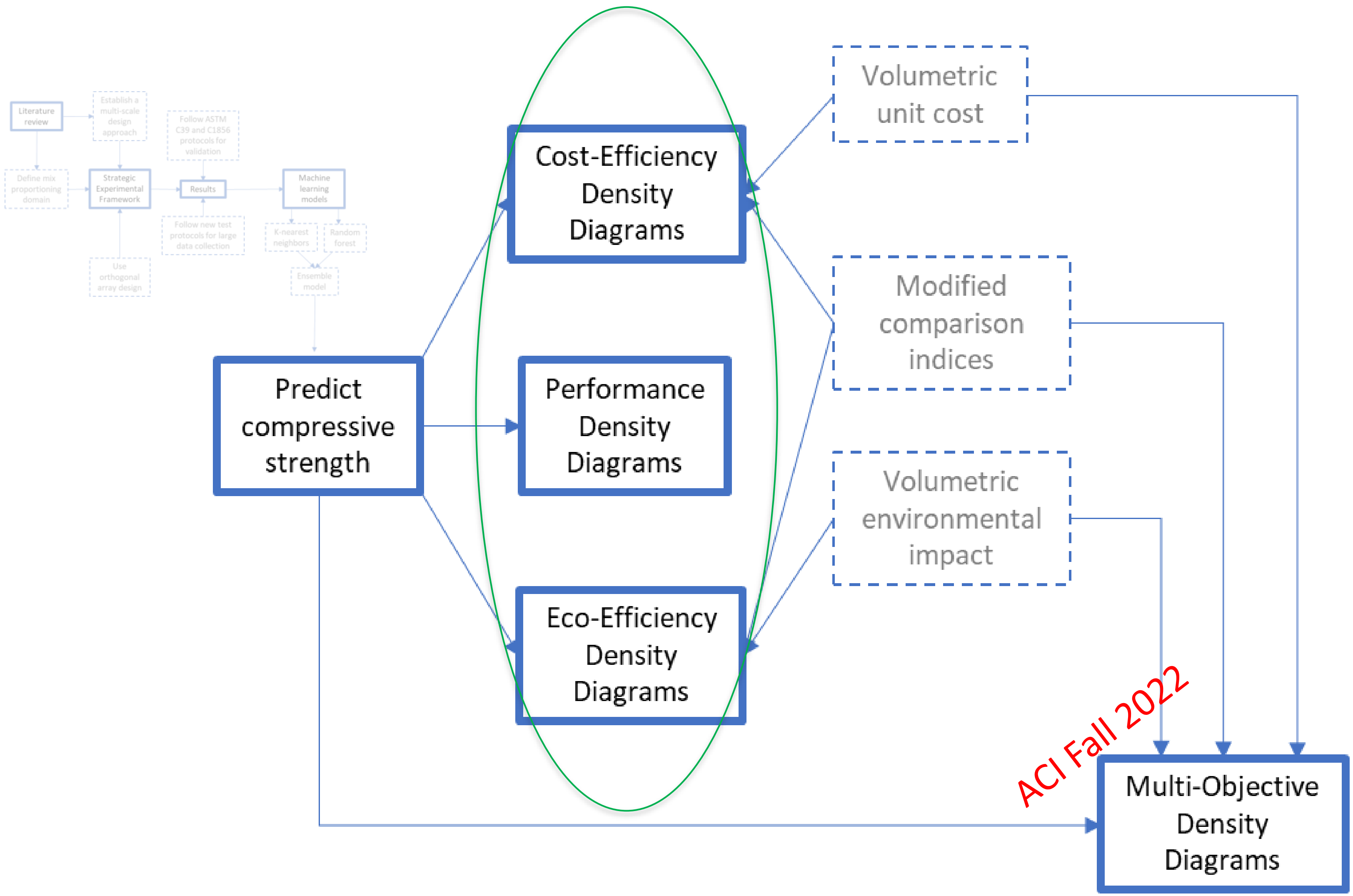




Phase A(I)						
Levels		1	2	3	4	5
Features	Slag	0	15	30	45	60
	Microsilica	0	5	10	15	20
	Fly Ash	0	3.75	7.5	11.25	15


Literature review
Establish a multi-scale design approach
Define mix proportioning domain
Strategic Experimental Framework
Use orthogonal array design
Results
Machine learning models
K-nearest neighbors
Random forest
Ensemble model
Predict compressive strength


Volumetric unit cost
Cost-Efficiency Density Diagrams
Modified comparison indices
Predict compressive strength
Performance Density Diagrams
Volumetric environmental impact
Eco-Efficiency Density Diagrams
Multi-Objective Density Diagrams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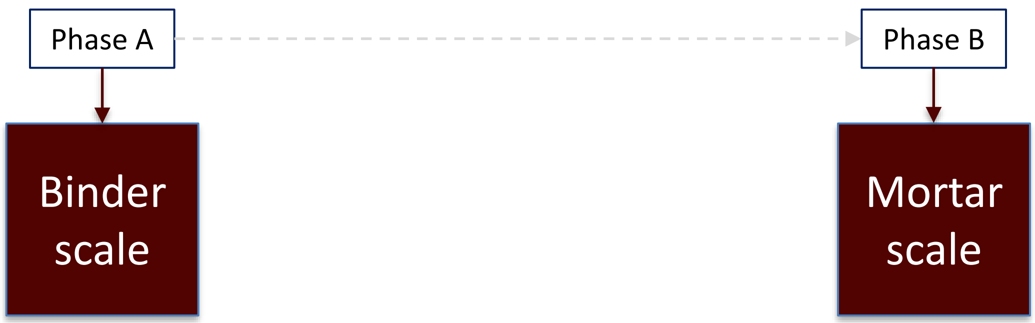
ACI Fall 2022

METHODOLOGY

Design strategy

Design strategy



Design strategy

Phase A → **Binder scale**

Variables:
- Slag
- Microsilica
- Fly ash
- w/cm
- HRWR/cm

Phase B → **Mortar scale**

Variables:
- Concrete sand
- Crushed sand
- Ground Quartz
- w/cm
- HRWR/cm

Orthogonal array variables: Slag, Microsilica, Fly ash (Phase A); Concrete sand, Crushed sand, Ground Quartz (Phase B)

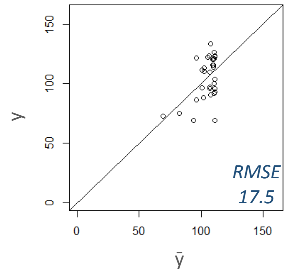
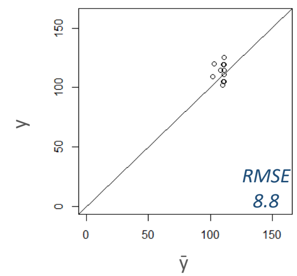
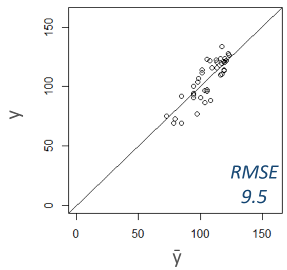
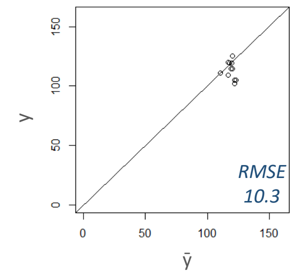
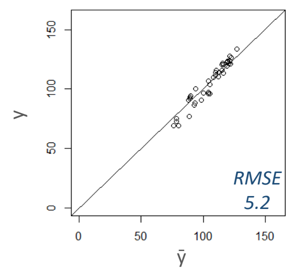
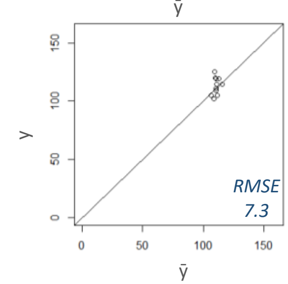
MODELING

Modeling

Methods/algorithms:

- kNN
- Random Forest
- Linear regression (polynomial models)

Modeling

Model	Train set	Optimum Test set
poly3_avg_84_Phase A(I)+A(II) with 3 variables		
✓ kNN_avg_100_Phase A(I)+A(II) with 4 variables *Cross validation RMSE 12.8*		
✓ RF_avg_100_Phase A(I)+A(II) with 4 variables *Bootstrap aggregation RMSE 12.8*		

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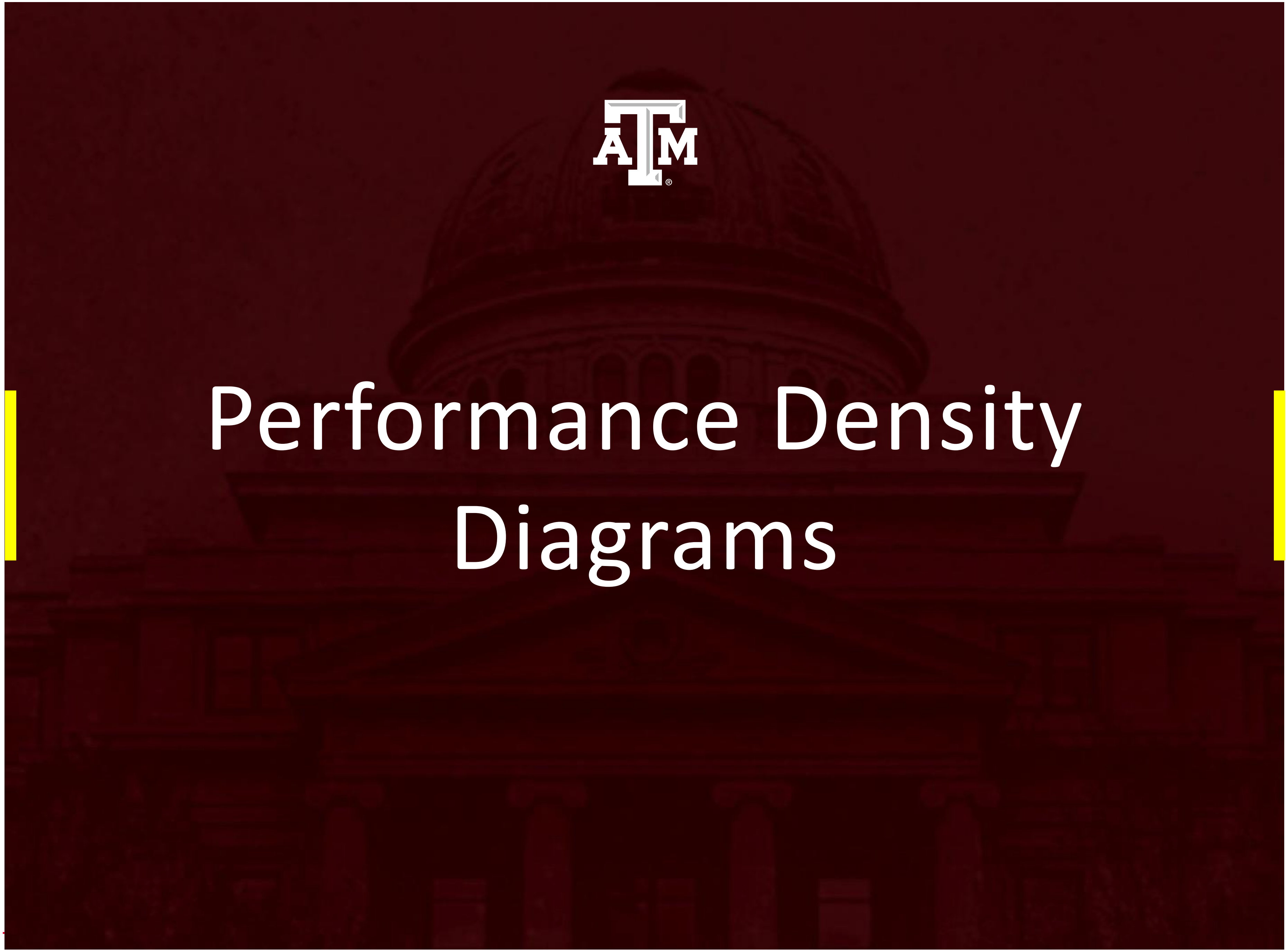
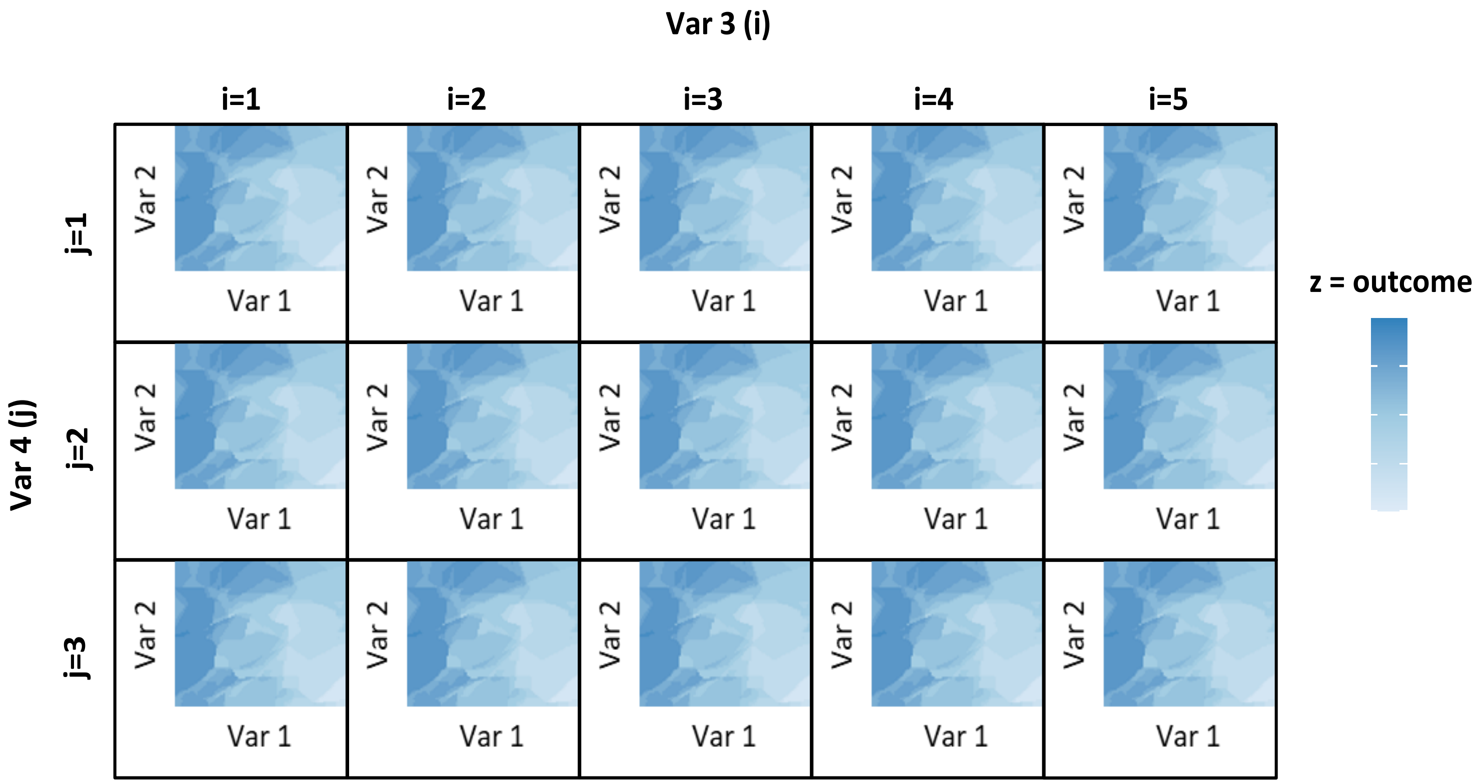
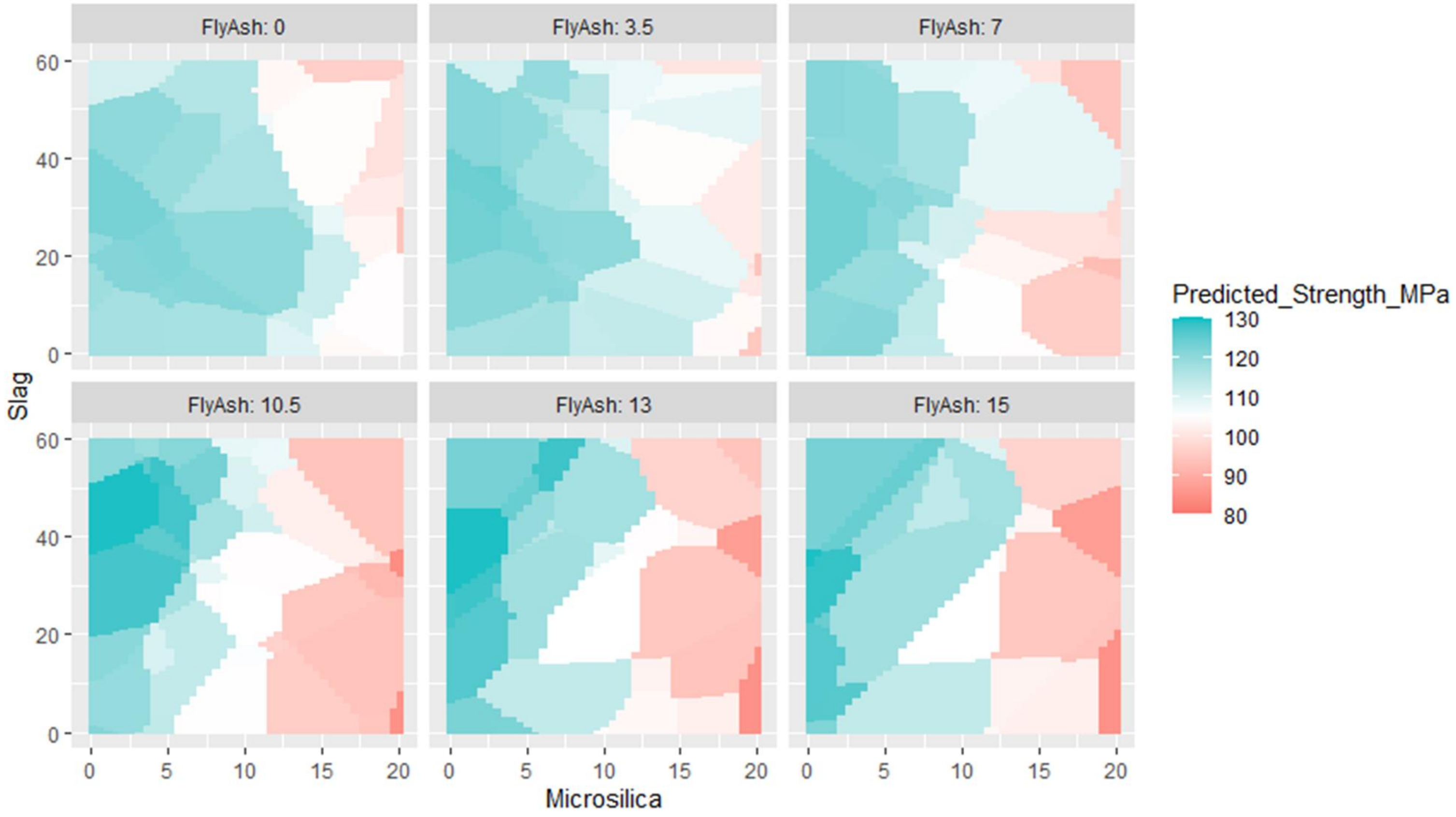

Performance Density
Diagrams

PDD



PDD

1. Use to optimize a certain material property (e.g., fc = 130 MPa)



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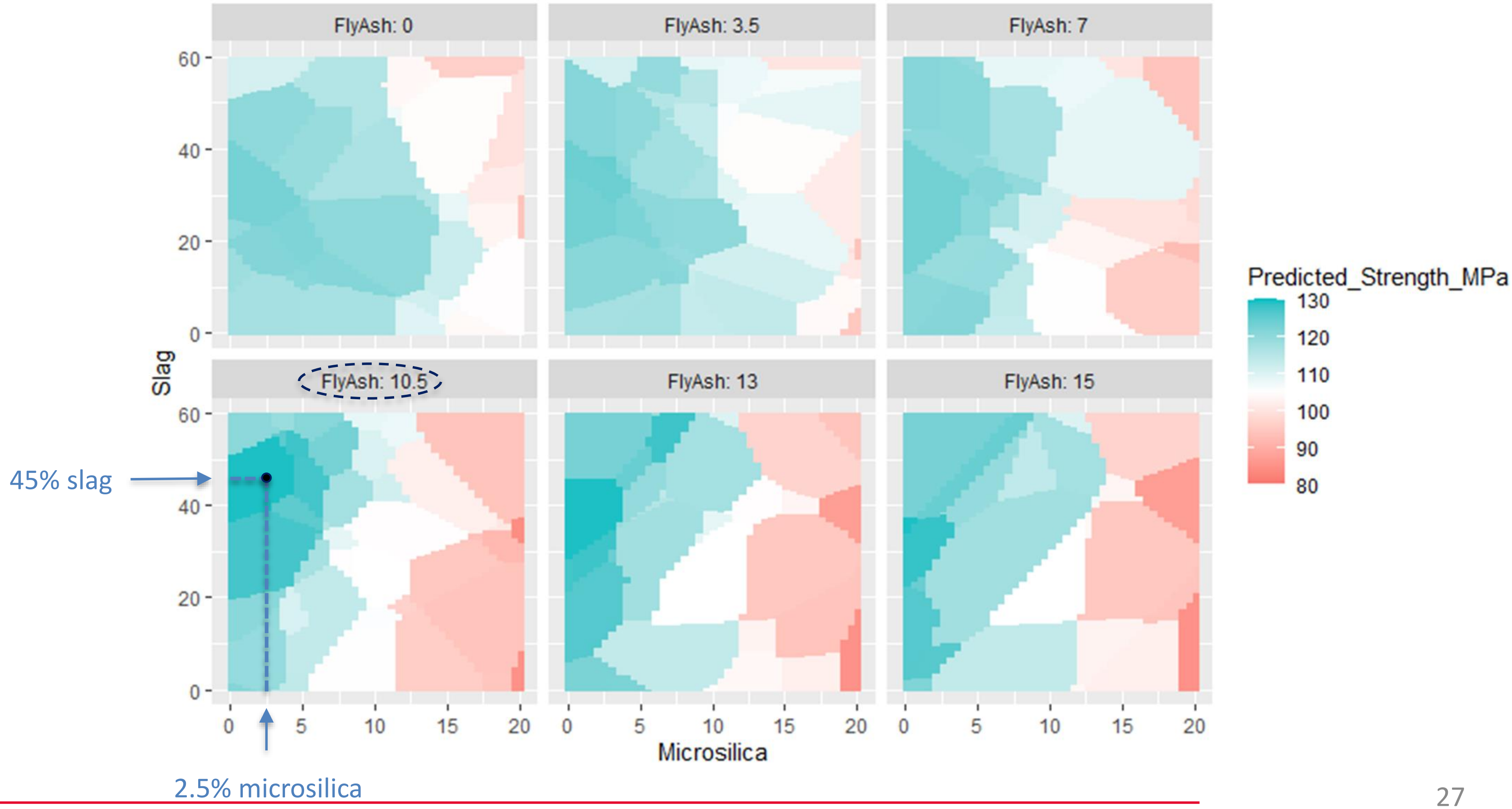
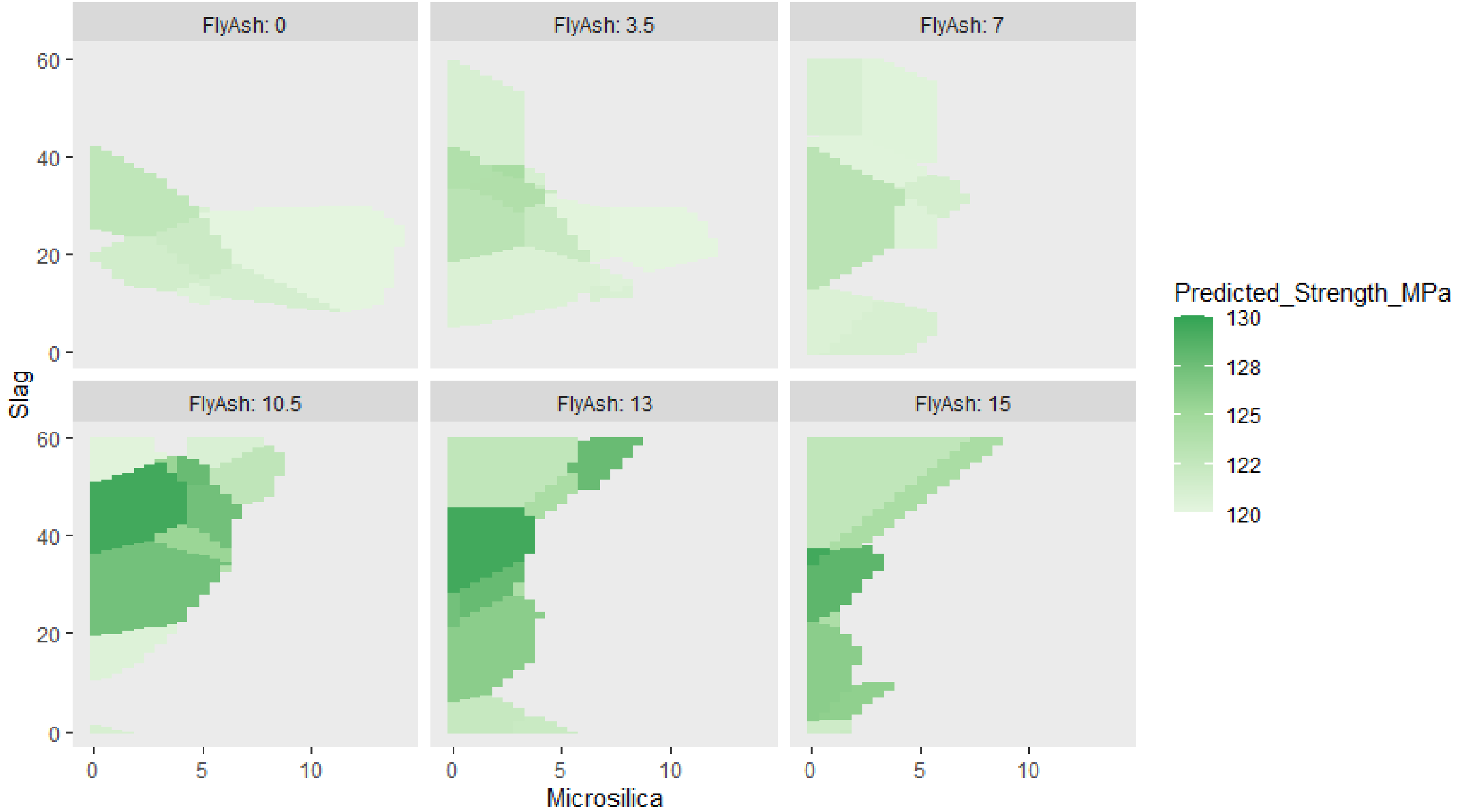


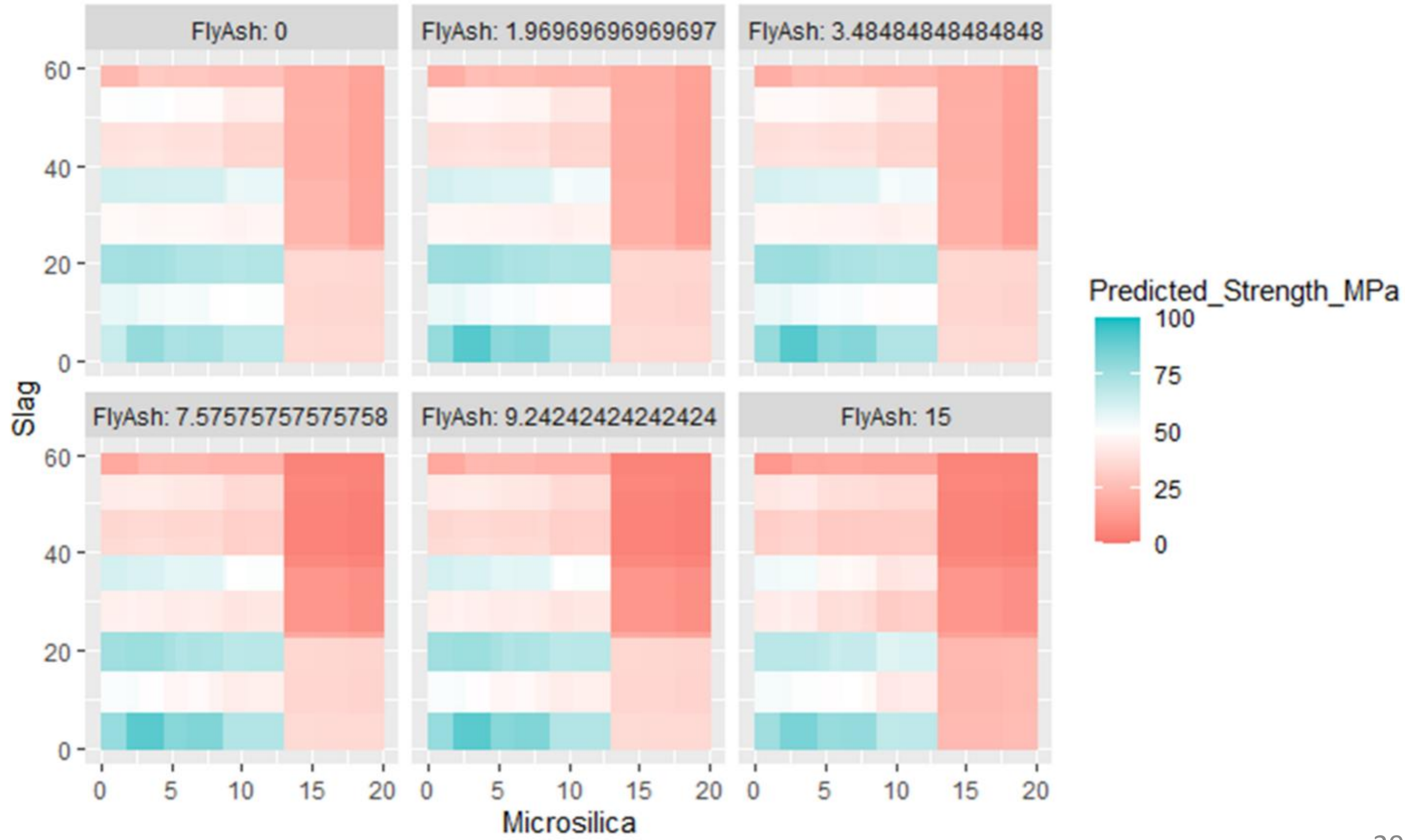
PDD

2. Impose design limits and evaluate alternative mixtures (e.g., fc > 120 MPa)



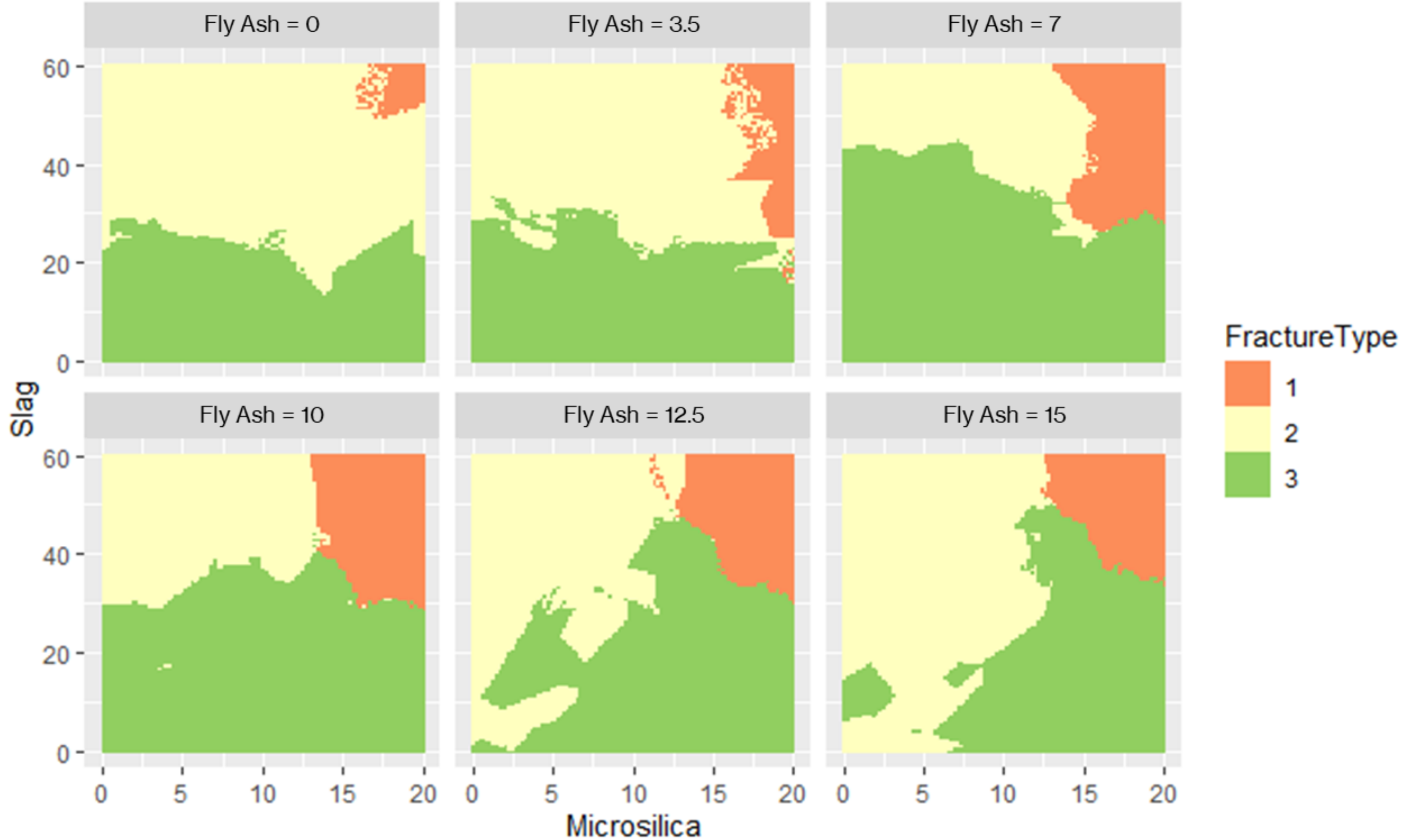
PDD

3. Use to evaluate predictive structure of models -> detect errors



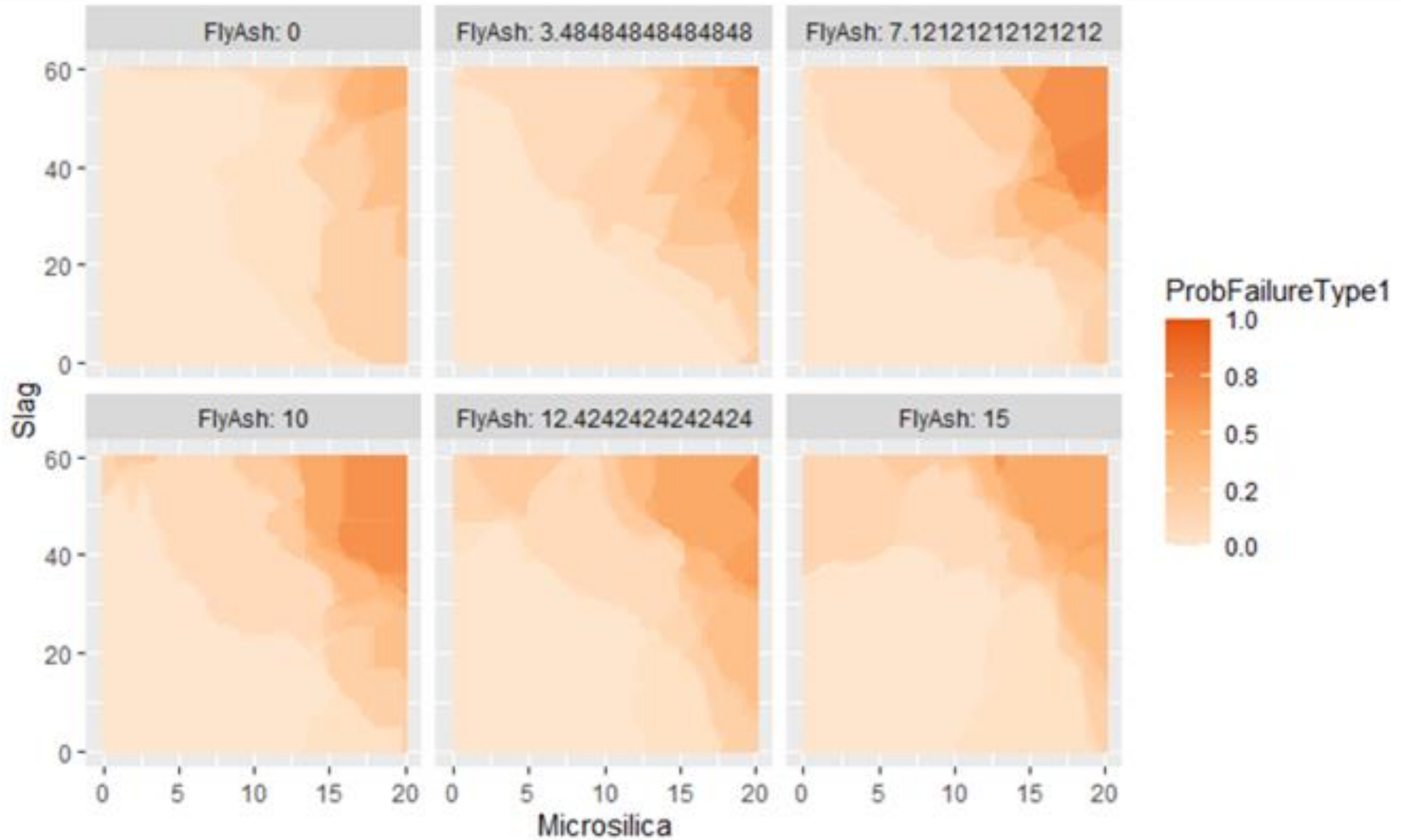
PDD

4. Make categorical predictions -> e.g., failure models



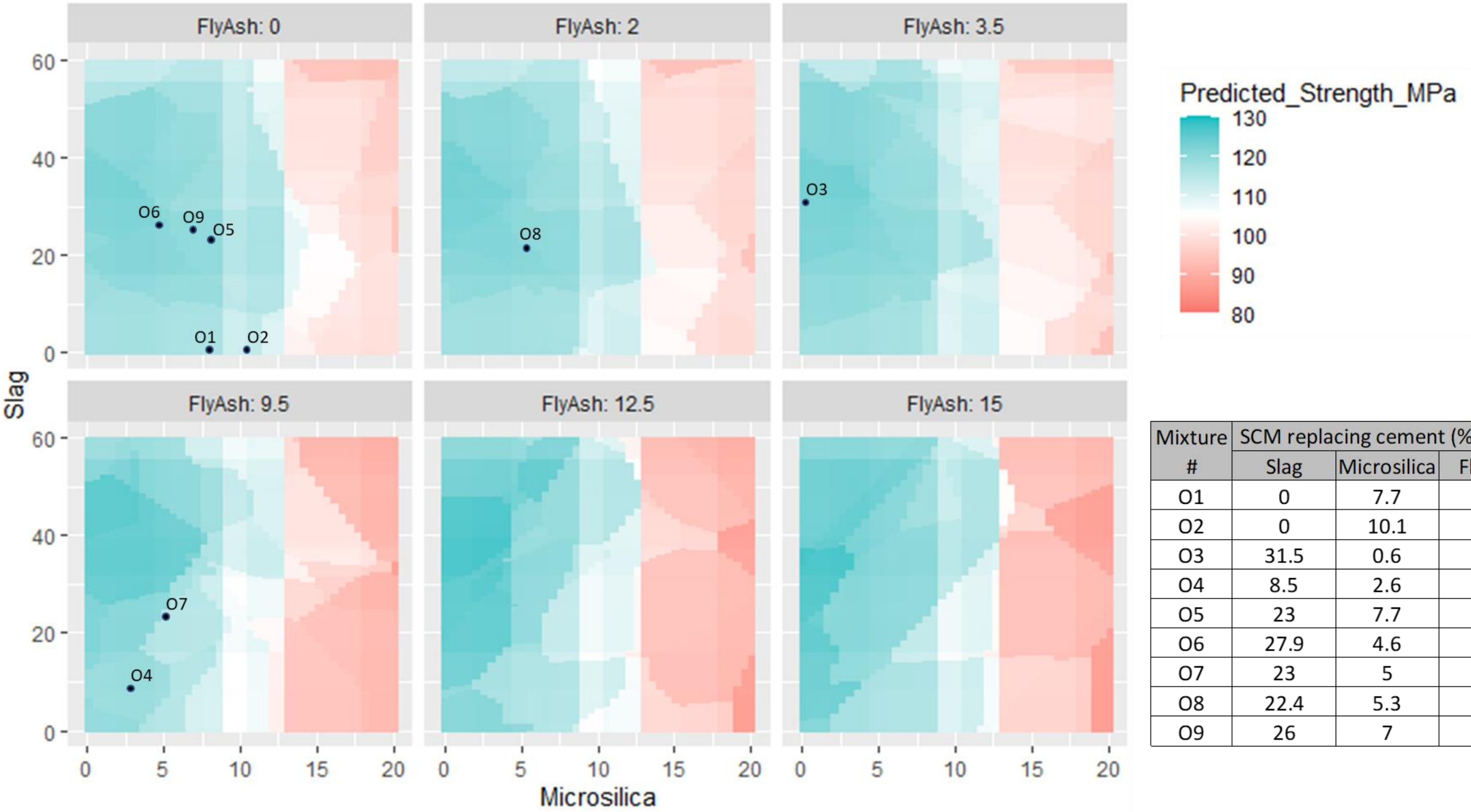
PDD

5. Evaluate probability of failure occurrences with Categorical PDDs



Results

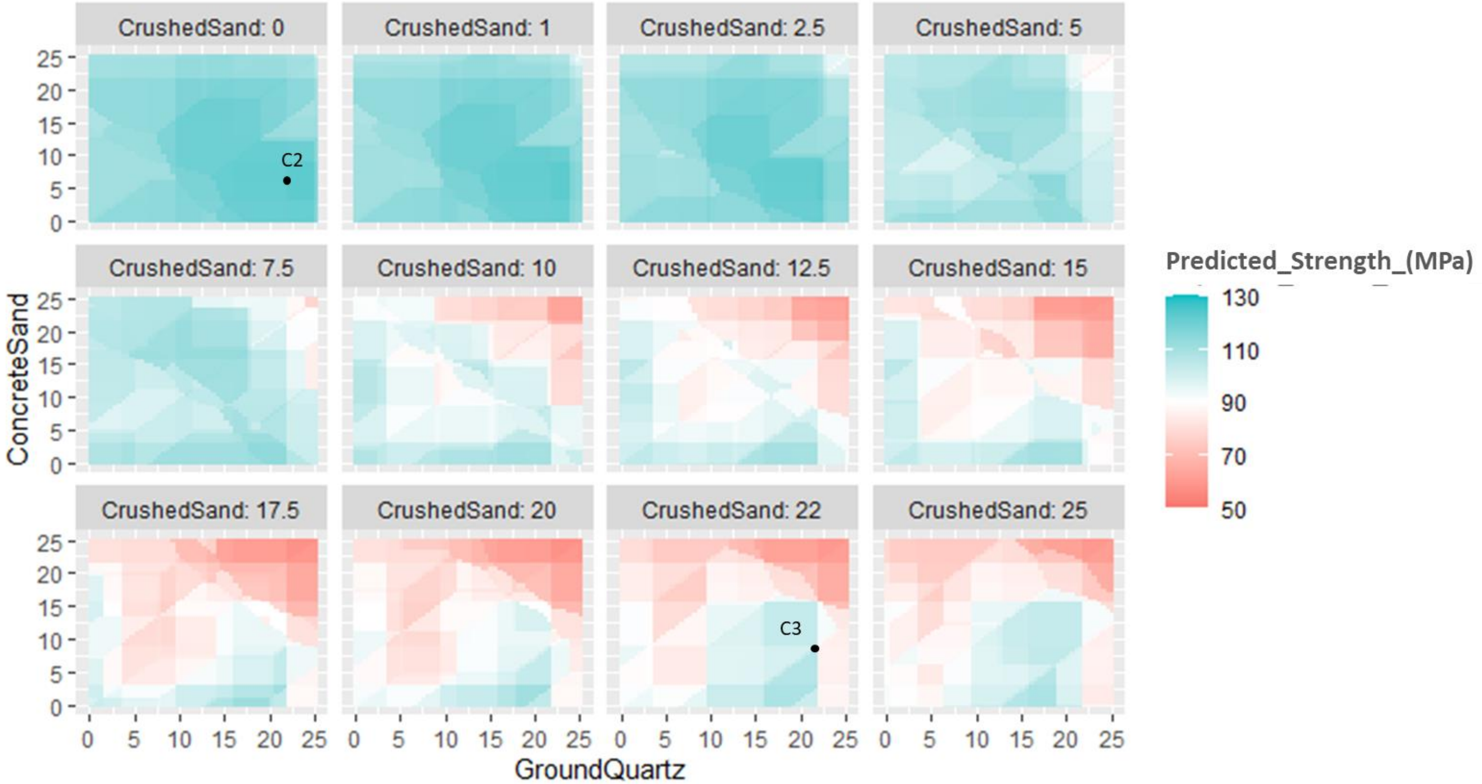
PDD Phase A



Mixture #	SCM replacing cement (% by wt) Slag	Microsilica	Fly Ash	fc (MPa) 56 days
O1	0	7.7	0	109
O2	0	10.1	0	120
O3	31.5	0.6	3.5	105
O4	8.5	2.6	9.2	114
O5	23	7.7	0	119
O6	27.9	4.6	0.5	126
O7	23	5	9.4	111
O8	22.4	5.3	2	105
O9	26	7	0	119

PDD

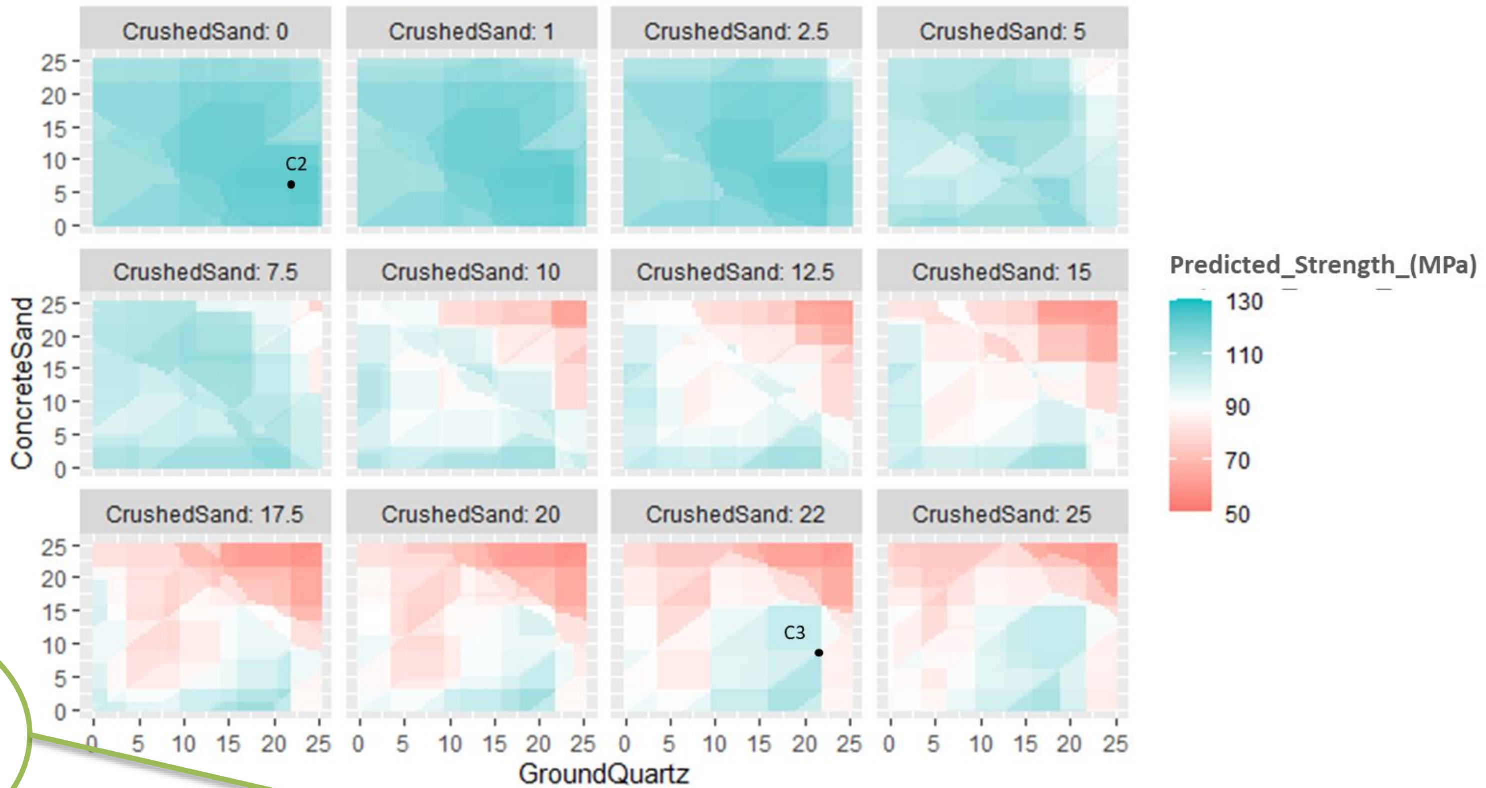
Phase B



Mixture #	SCM replacing cement (% by wt)			Aggregates replacing cementitious (% by wt)			56 day results	
							New test method	ASTM C1856
	Slag	Microsilica	Fly Ash	Ground Quartz	Concrete Sand	Crushed Sand	f'c (MPa)	f'c (MPa)
C1	0	10.1	0	22	6.5	0	128.4	133.8
C2	22.4	5.25	1.97	22	6.5	0	129.2	158.1
C3	22.4	5.25	1.97	21.5	8.5	22	128.5	154.8

PDD

Phase B



C3
fc = 155 MPa
Fa/cm > 1

Mixture #	SCM replacing cement (% by wt)			Aggregates replacing cementitious (% by wt)			56 day results	
							New test method	ASTM C1856
	Slag	Microsilica	Fly Ash	Ground Quartz	Concrete Sand	Crushed Sand	f'c (MPa)	f'c (MPa)
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Cost and Environmental Impact

Eco-efficiency Indices

[1] $$\chi_{column} = \frac{i_c}{f_c}$$

[1],[2] $$\chi_{cracking} = \lambda_{fr} \left(\frac{i_c}{f_c^{\ 0.25}} \right)$$

f_c Compressive strength (MPa)

λ_{fr} Coefficient for modulus of rupture $\lambda_{fr} = 1.1125 e^{-0.004 f_c}$

i_c Volumetric environmental impact (kg $CO_{2\text{-}eq}/m^3$)

[1] proposed by Kourehpaz and Miller (Kourehpaz and Miller 2019)
[2] proposed modification in this work

Cost-efficiency Indices

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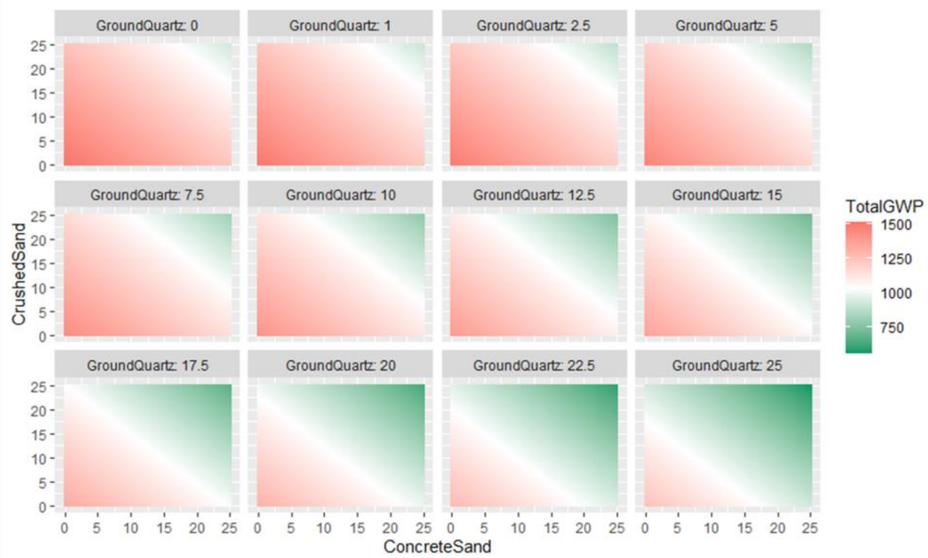
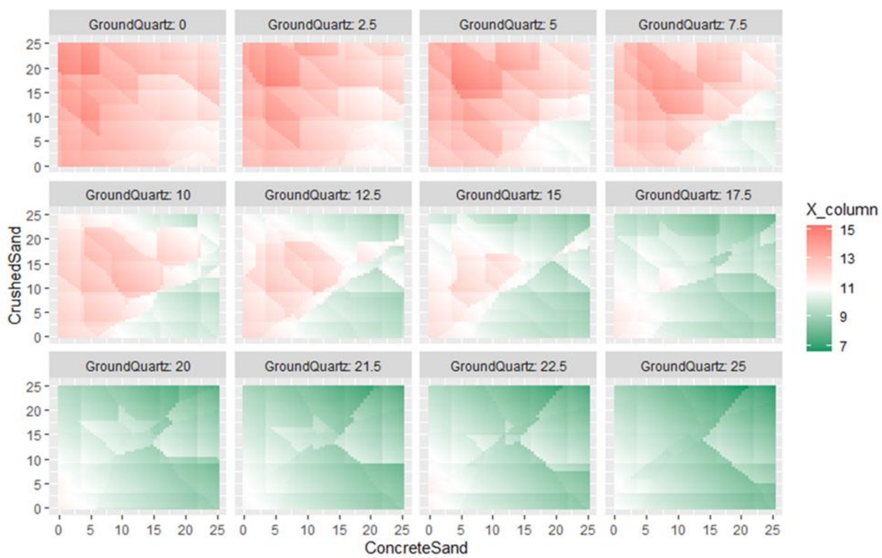
u_c Volumetric unit cost ($/m^3)

Volumetric environmental impact vs Eco-Efficiency Density Diagrams

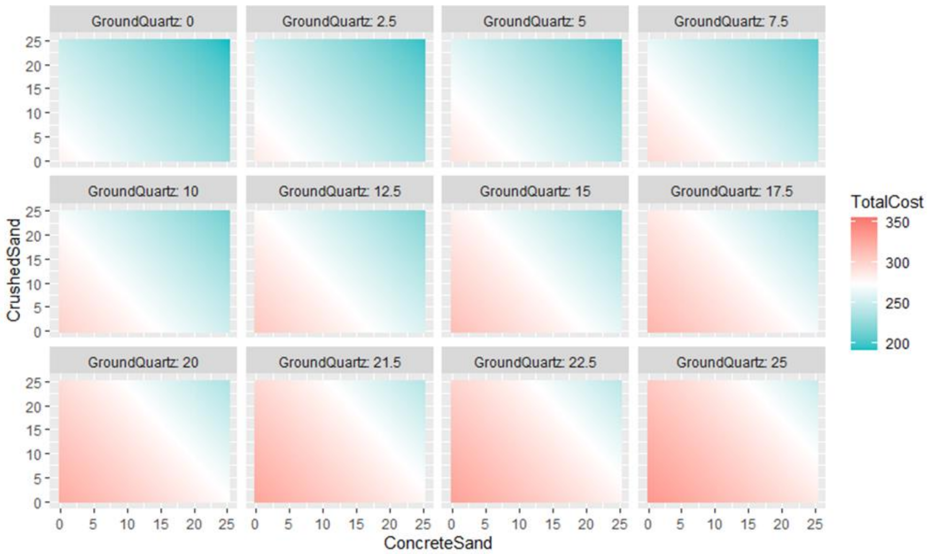


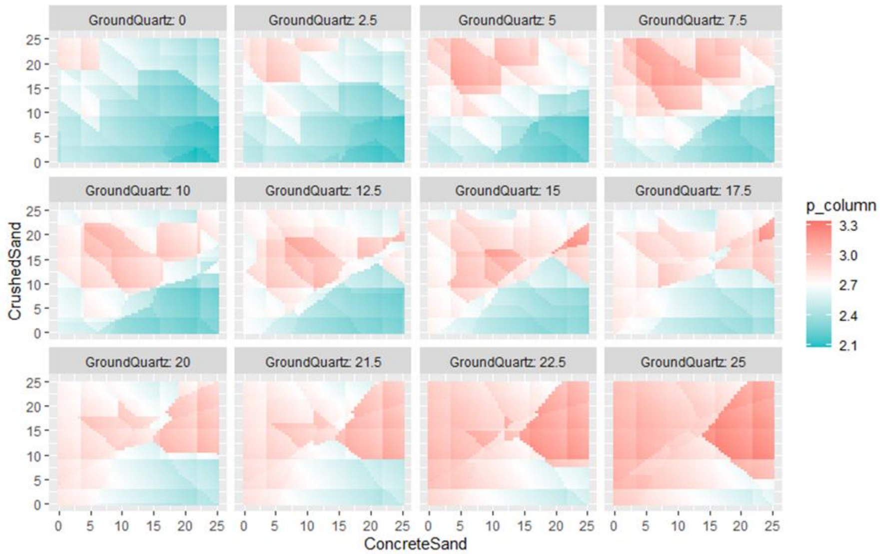


$$TotalGWP = i_c(ingredientA) + i_c(ingredientB) + \ldots$$

(kg $CO_{2\text{-eq}}/m^3$)

Volumetric Unit Cost vs Cost-Efficiency Density Diagrams





Volumetric Indicators vs Efficiency Indicators

Mix #	Description	aggregates (% by wt) replacing cementitious content: concrete sand	crushed sand	ground quartz	Total Cost ($/m³)	ρ_column	fc (MPa)
ρ-Col-1	with min(ρ_column)	21.5	2.5	0	233	2.08	112
ρ-Col-2	with min(Total Cost)	25	25	0	190	2.37	80
ρ-Col-3	same ρ_column ρ-Col-2 & higher cost	11	2.5	11.5	279	2.37	118
ρ-Col-4	with lowest predicted strength	22	17.5	14	240	3.21	74.8
ρ-Col-5	with highest predicted strength	9.5	0	19	303	2.56	118
					Total GWP (kg CO_2-eq/m³)	χ_column	fc (MPa)
χ-Col-1	with min(χ_column)	20.5	25	25	625	6.58	95
χ-Col-2	with min(Total GWP)	25	25	25	552	6.75	82
χ-Col-3	same χ_column as χ-Col-2 & higher GWP	19.5	25	25	641	6.75	95
χ-Col-4	with lowest predicted strength	22	17.5	14	875	11.70	74.8
χ-Col-5	with highest predicted strength	9.5	0	19	1197	10.10	118

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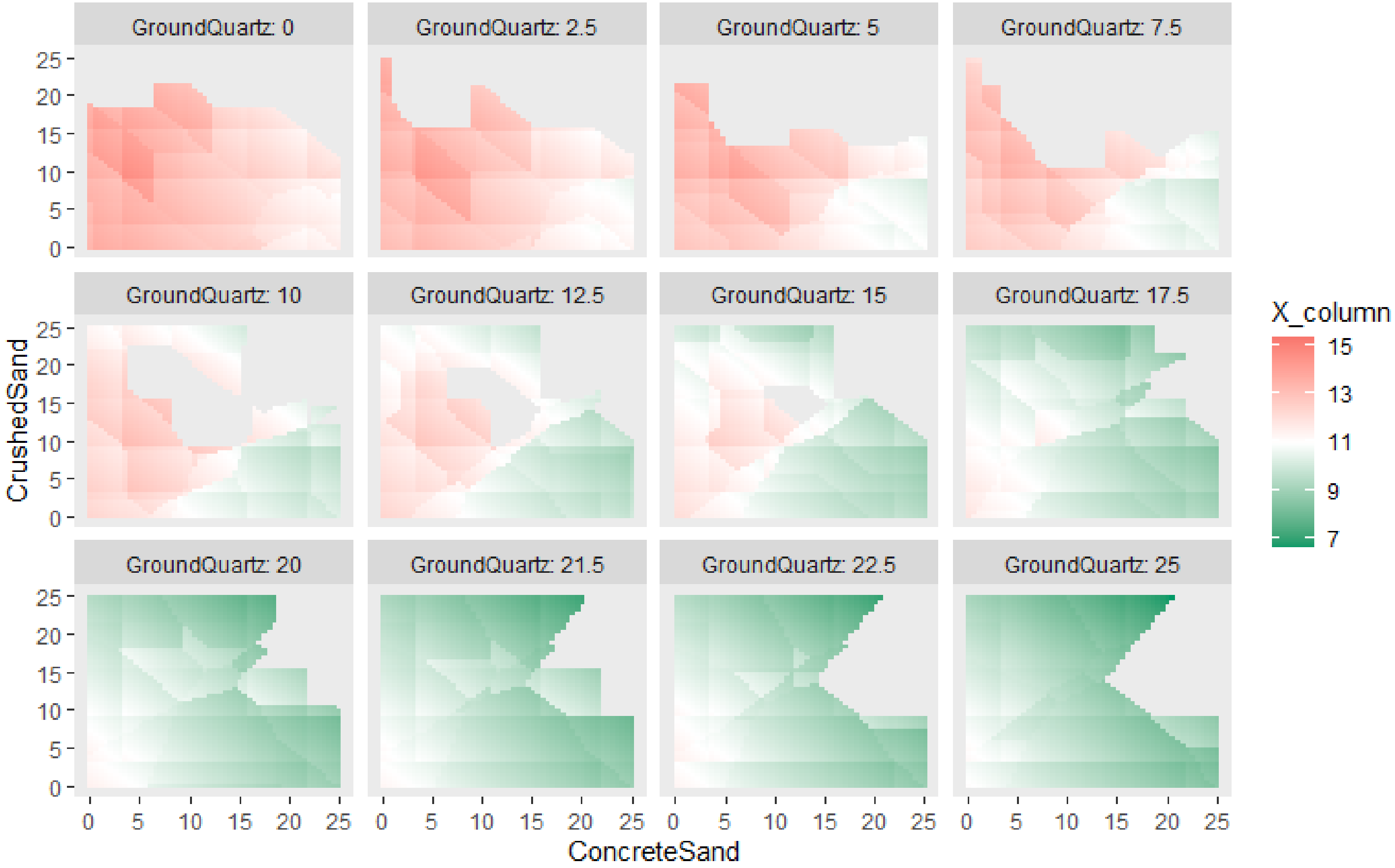
Filtered Eco-Efficiency Density Diagrams



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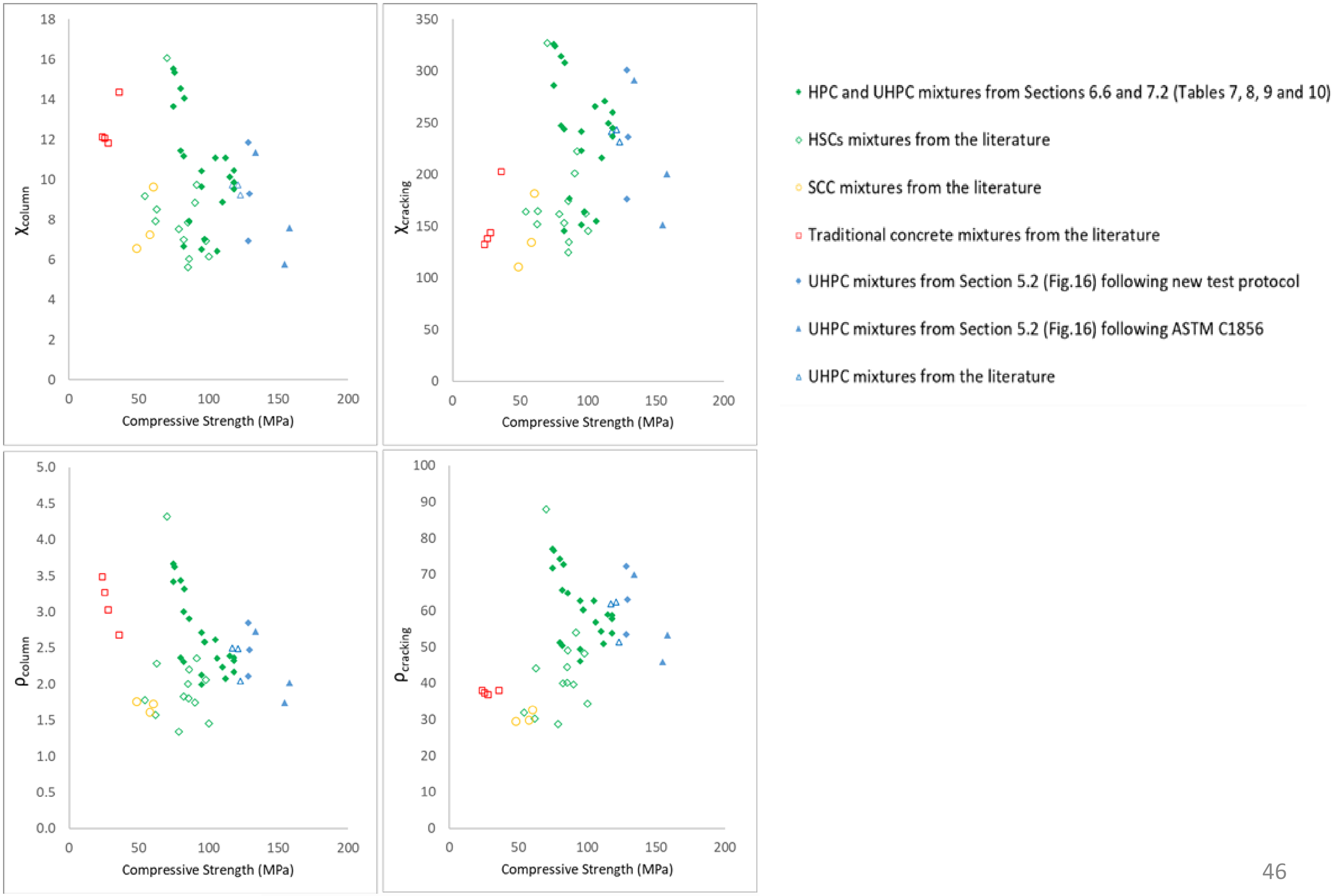
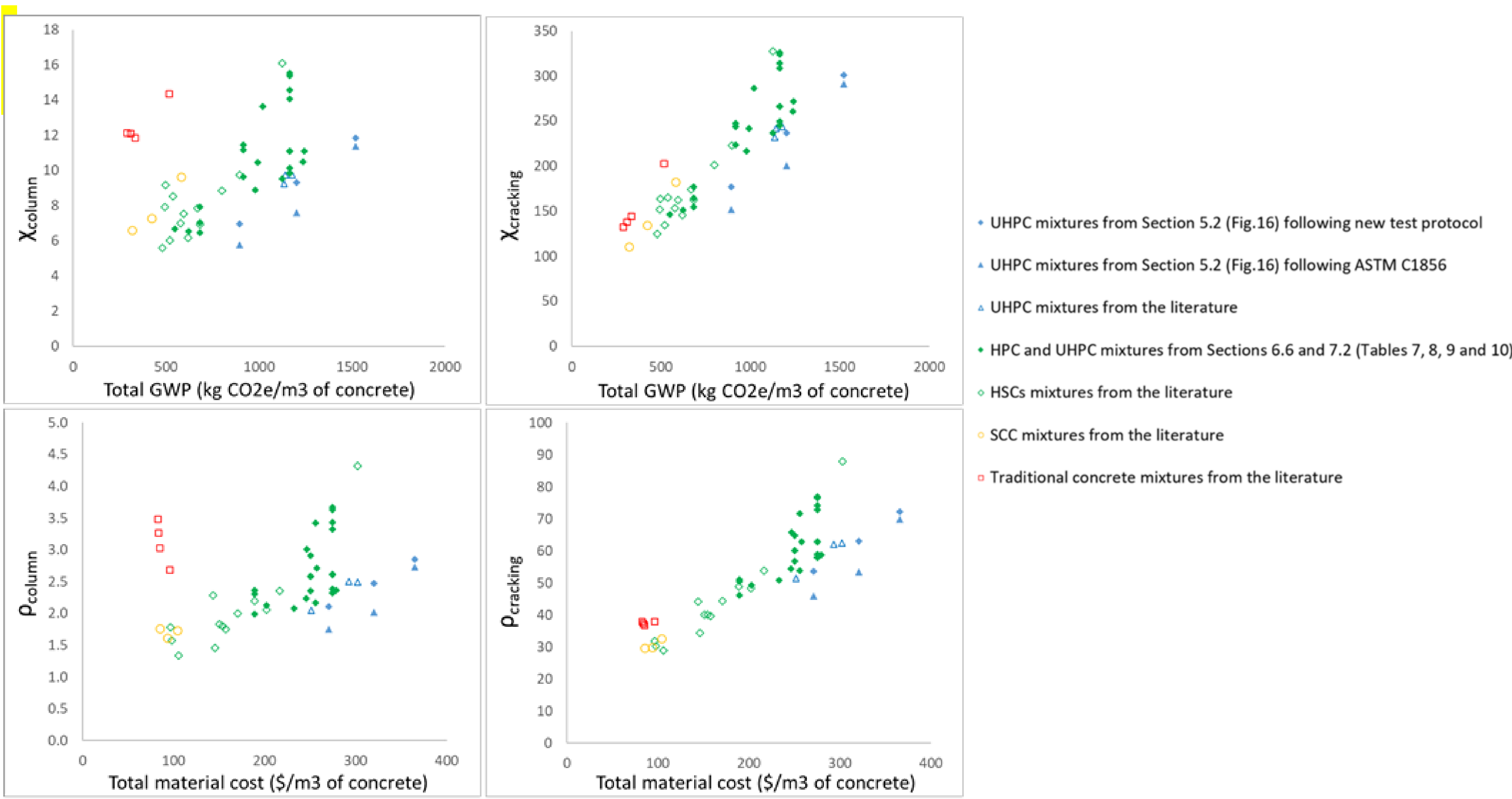
COMPARISON BETWEEN DIFFERENT CONCRETE TECHNOLOGIES



χ_{column}
Compressive Strength (MPa)
$\chi_{cracking}$
Compressive Strength (MPa)
ρ_{column}
Compressive Strength (MPa)
$\rho_{cracking}$
Compressive Strength (MPa)
HPC and UHPC mixtures from Sections 6.6 and 7.2 (Tables 7, 8, 9 and 10)
HSCs mixtures from the literature
SCC mixtures from the literature
Traditional concrete mixtures from the literature
UHPC mixtures from Section 5.2 (Fig.16) following new test protocol
UHPC mixtures from Section 5.2 (Fig.16) following ASTM C1856
UHPC mixtures from the literature


χcolumn
Total GWP (kg CO2e/m3 of concrete)
χcracking
Total GWP (kg CO2e/m3 of concrete)
ρcolumn
Total material cost ($/m3 of concrete)
ρcracking
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CONCLUSIONS

1. Can we accurately estimate the compressive strength of UHPC with reduced experimental runs & ML models? -> **YES (OA+ML)**

2. Can we evaluate the effect of changes in mix proportioning on mechanical performance in an easy and intuitive way? -> **YES (PDD)**

3. Can we evaluate the effect of mix proportioning & mechanical performance on cost and eco-efficiency concurrently? -> **YES (CEDD & EEDD)**

4. Are high paste content, high strength (and ultra-high strength) concrete technologies detrimental to cost and/or eco efficiencies? -> **NO**

IMPLICATIONS

Implications

- This study provides guidance -> develop EEDDs -> proof of optimization -> EPDs
- Facilitate decision making (material availability, cost, accessibility, embodied CO2)
- Facilitate communication between non-expert personnel (in AI and materials) involved in projects (owners, policy makers, designers, architects and producers)
- Lift mis-conceptional barriers on UHPC -> promote application where suitable
- Encourage innovative mix designs with new materials (e.g., nanomaterials)

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FUTURE WORK

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- New indices -> CO_2 of reinforcing steel on eco-efficiency
- New indices -> difference in span achieved in bridge elements (beams, girders) for different concretes -> weight of the superstructure -> number and volume of supporting substructural elements (columns, footing and piles)
- PDDs to optimize material properties other than compressive strength should be explored (e.g., fiber reinforced concretes)

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- Further improvement of the end-specimen conditions -> strengths over 125 MPa
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- New indices -> difference in span achieved in bridge elements (beams, girders) for different concretes -> weight of the superstructure -> number and volume of supporting substructural elements (columns, footing and piles)
- PDDs to optimize material properties other than compressive strength should be explored (e.g., fiber reinforced concretes)

Future Work

- New models -> inputs related to individual particle make-up (fineness, characteristic particle size and compound composition of the raw ingredients) -> potential to overcome the multi-source variability issue
- Inclusion of nanomaterials & fibers should be evaluated through standard test protocols -> compare UHPCs w/ much higher strengths vs other concretes

Future Work

- New models -> inputs related to individual particle make-up (fineness, characteristic particle size and compound composition of the raw ingredients) -> potential to overcome the multi-source variability issue

- Inclusion of nanomaterials & fibers should be evaluated through standard test protocols -> compare UHPCs w/ much higher strengths vs other concretes

Upcoming Publications

C. Tavares, *Multi-Objective Density Diagrams Developed with Machine Learning Models to Optimize Sustainability and Cost-Efficiency of UHPC Mix Design*, Ph.D. dissertation, Texas A&M University (May 2022)

C. Tavares, X. Wang, S. Saha, Z. Grasley, *Machine Learning-Based Mix Design Tools to Minimize Carbon Footprint and Cost of UHPC. Part 1: Efficient Data Collection and Modeling (*under review 2022)

C. Tavares and Z. Grasley, *Machine Learning-Based Mix Design Tools to Minimize Carbon Footprint and Cost of UHPC. Part 2: Cost- and Eco-Efficiency Density Diagrams (*under review 2022)

References

Kourehpaz, Pouria, and Sabbie A. Miller. 2019. 'Eco-efficient design indices for reinforced concrete members', *Materials and Structures*, 52: 96.

THANK YOU!

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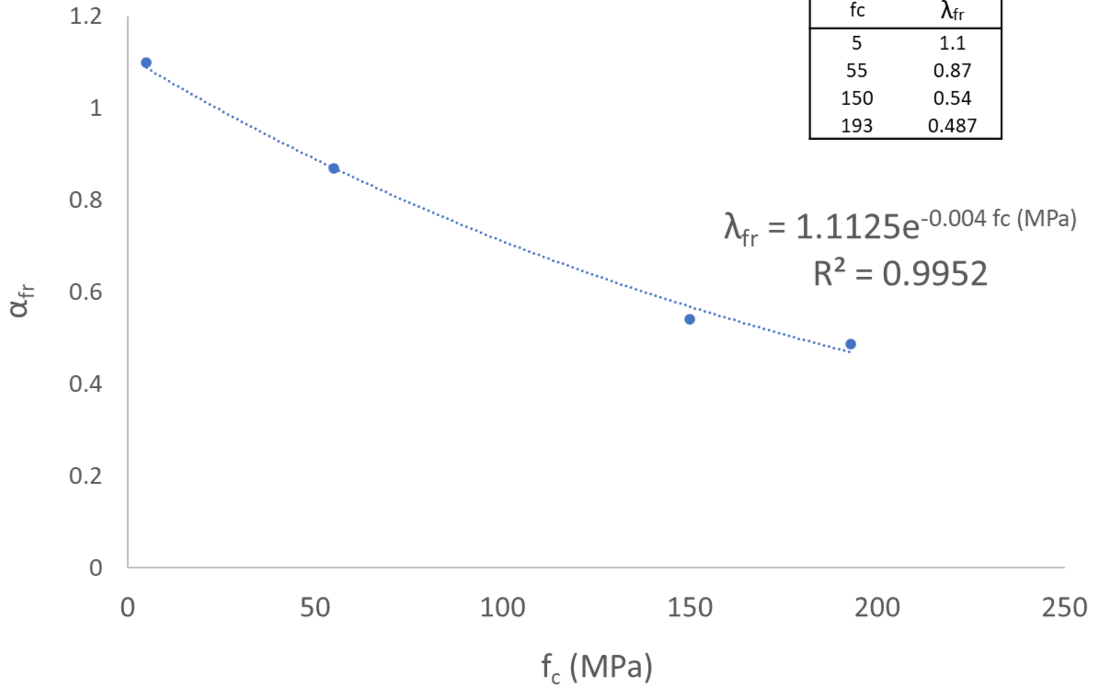
APPENDIX



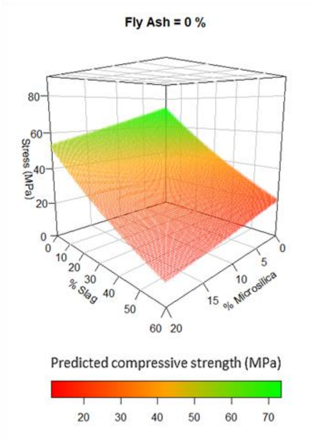
fc	λ_{fr}
5	1.1
55	0.87
150	0.54
193	0.487

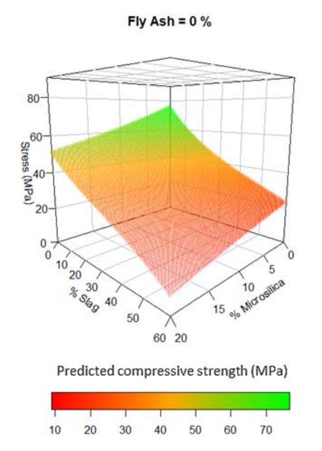
$$f_r = 0.62\sqrt{f_c(MPa)}$$

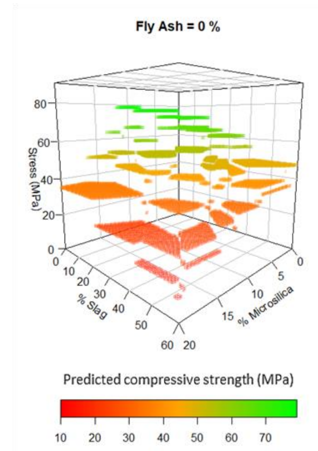
$$f_r = 0.94\sqrt{f_c(MPa)}$$

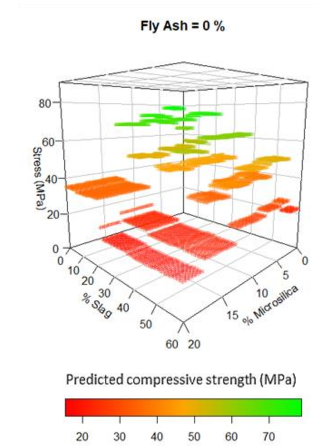
$$f_r = 2.55\sqrt{f_c(MPa)}$$

3D density plots -> predictive structure





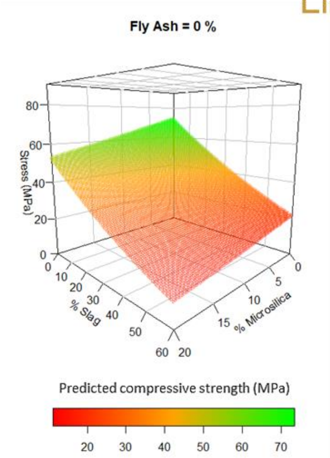


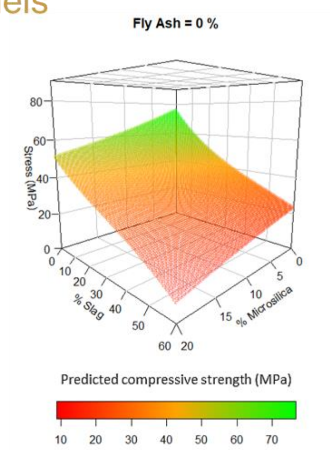


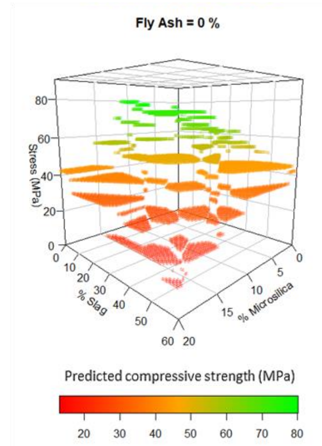
Linear Models

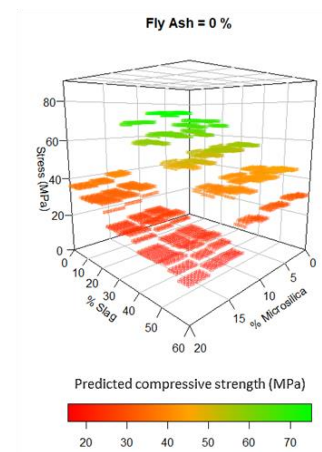
kNN Models

RF Models

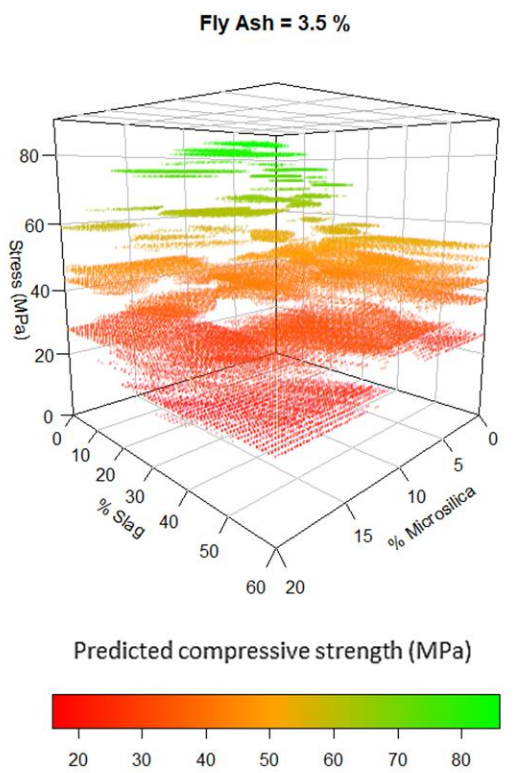






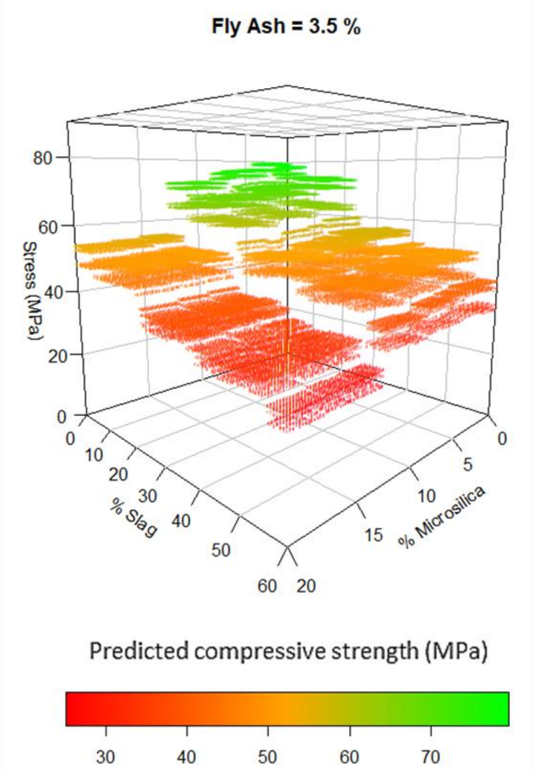


Modeling



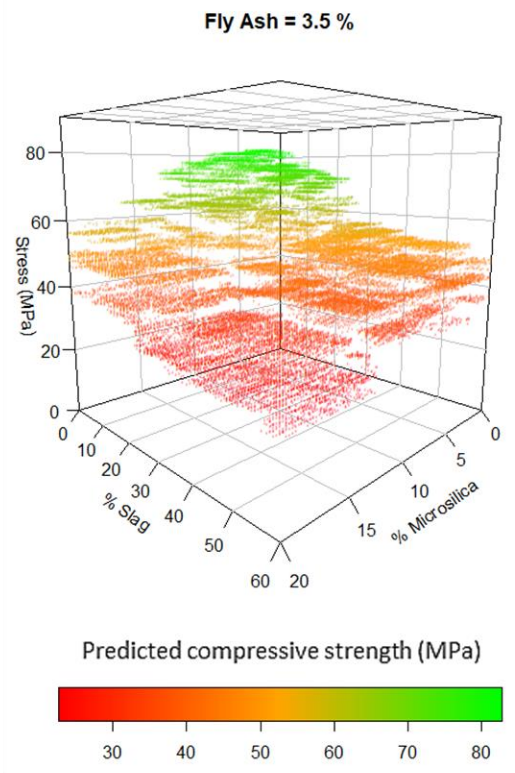
kNN Model

+



RF Model

=



Ensemble Model

Modeling

Evaluating predictive performance of models:

- 3D density plots
- ***RMSE***
- ***Correlation plots (predictions vs actual outcomes)***

R^2 is only applicable to evaluate linear regression*

*Spiess and Neumeyer, *An evaluation of R^2 as an inadequate measure for nonlinear models in pharmacological and biochemical research: a Monte Carlo approach*

Eco-efficiency Indices

$$\sigma = \frac{M * c}{I_x} \dashrightarrow fr = \frac{6M}{bh^2}$$

$$M_c = \frac{f_r bh^2}{6} \quad \text{vs} \quad M_{\max} = \frac{wl^2}{8}$$

$$h = 0.866 \frac{w^{0.5} l}{b^{0.5} f_r^{\ 0.5}}$$

Eco-efficiency Indices

$$h = 0.866 \frac{w^{0.5} l}{b^{0.5} f_r^{0.5}}$$

$$\tilde{I} = l(bh - A_s) i_c + l A_s i_s$$

ACI 318 building code (NSC): fc < 55MPa $f_r = 0.62\sqrt{f_c(MPa)}$

ACI 363 (HSC): fc > 55MPa $f_r = 0.94\sqrt{f_c(MPa)}$

ACI 239 (UHPC): fc >150 MPa $f_r = 2.55\sqrt{f_c(MPa)}$

$$\lambda_{fr} = 1.1125 e^{-0.004 f_c}$$

$$\tilde{I} = l^2 (wb)^{0.5} \lambda_{fr} \left(\frac{i_c}{f_c^{0.25}} \right) - l A_s i_c + l A_s i_s$$

Eco-efficiency Indices

$$\tilde{I} = l^2 (wb)^{0.5} \lambda_{fr} \left(\frac{i_c}{f_c^{\,0.25}} \right) - l A_s i_c + l A_s i_s$$

$$\chi_{cracking} = \lambda_{fr} \left(\frac{i_c}{f_c^{\,0.25}} \right)$$