Apr 2nd, 2023

ACI Convention
San Francisco, CA

# From Data-Driven Models to Material Characterization: A New Approach to Improve Durability and Mechanical Performance of High-Early Strength Concretes

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# Decarbonization strategies in the cement and concrete industries

Habert, G., et al. "Environmental Impacts and Decarbonization Strategies in the Cement and Concrete Industries." *Nature Reviews Earth & Environment* 1.11 (2020): 559-73. Print.

| **Readily implementable solutions:** | **Long-term solutions:** |
| --- | --- |
| Efficiency of clinker production | Electrification of cement production |
| Efficiency of cement production | Alternative cements |
| Efficiency of concrete proportioning | Carbon sequestration |
| Efficiency of structural design | |

*Our Research focus*

Carbon sequestration: $CO_2$

# Decarbonization strategies in the cement and concrete industries

Habert, G., et al. "Environmental Impacts and Decarbonization Strategies in the Cement and Concrete Industries." *Nature Reviews Earth & Environment* 1.11 (2020): 559-73. Print.

## Readily implementable solutions:

Efficiency of clinker production

Efficiency of cement production

Efficiency of concrete proportioning

*Focus of this presentation*

*Sunday, April 2nd*
*3:30 – 5:30 PM,*
*Yosemite A*

Efficiency of structural design

## Long-term solutions:

Electrification of cement production

Alternative cements

$CO_2$

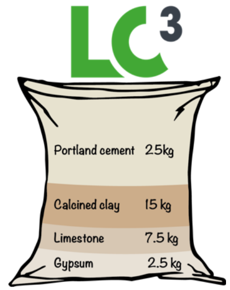
Carbon sequestration

# Motivation of this Study

# New green materials emerge everyday…

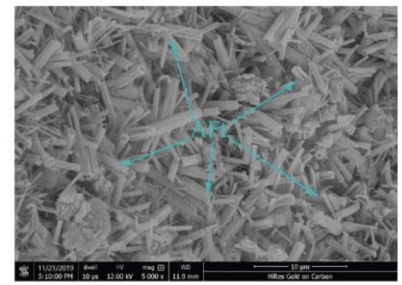
*Electrically produced cement*

http://sublime-systems.com/




http://lc3.ch/about-lc3/

*CSA cements*



https://www.hindawi.com/journals/amse/2021/4494056/

Challenges:
- Extensive studies to assess all performance needs
- Unknown long-term performance
- Limited data available for complex AI modeling

*Enzymatic self-healing cementitious material*

https://cen.acs.org/materials/Enzymes-power-carbon-sucking-alternative/100/i6
Credit: Shaui Wang, Suzanne Scarlata, Nima Rahbar

# Problem Statement

**Major Need:**

Efficient tools to **expedite the incorporation of new materials** into new and existing concrete formulations

Mixture Design
-> Optimization <-

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

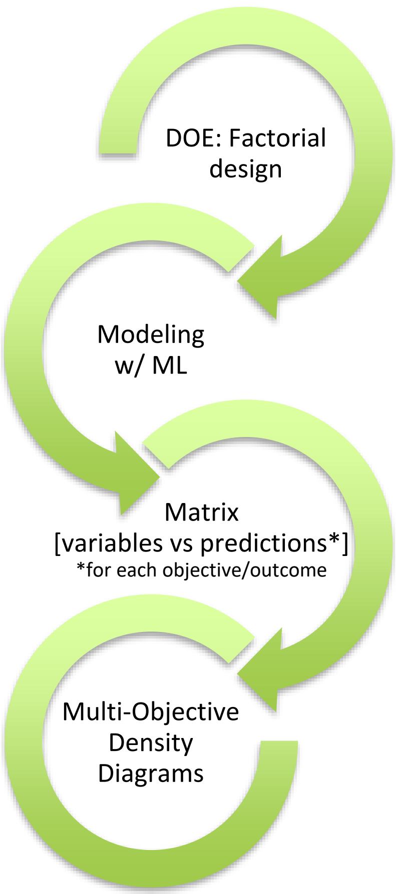
# Key questions addressed in this research

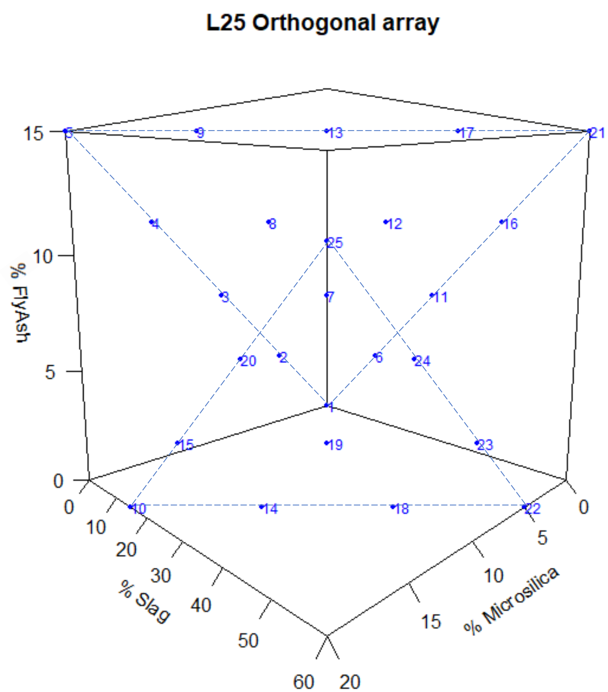
1. Can we effectively optimize concrete mix design w/ **few experimental runs**?

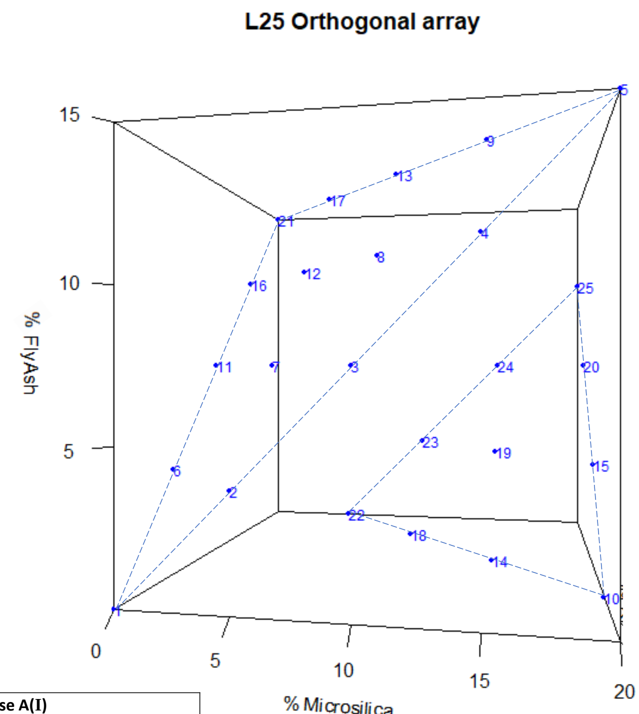
2. Can we evaluate: mechanical performance <- f(changes in mix proportion) in an easy and intuitive way?

# Optimization strategy

# Conceptual framework



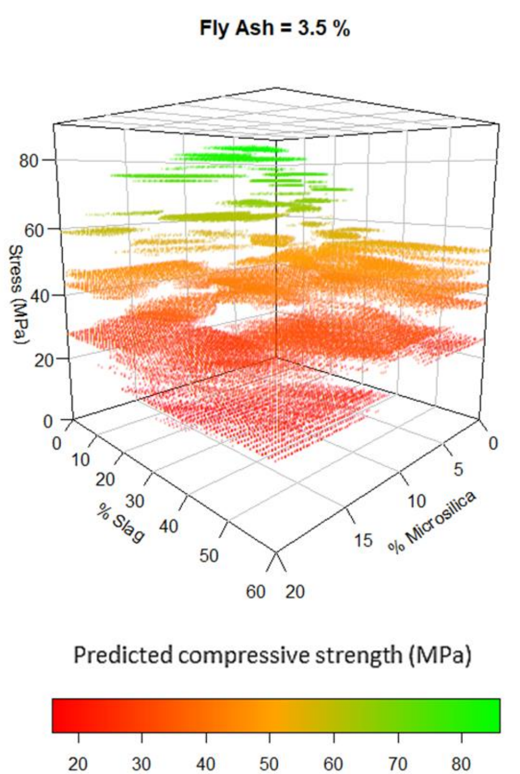

| Phase A(I) | | | | | | |
|---|---|---|---|---|---|---|
| Levels | | 1 | 2 | 3 | 4 | 5 |
| Features | Slag | 0 | 15 | 30 | 45 | 60 |
| | Microsilica | 0 | 5 | 10 | 15 | 20 |
| | Fly Ash | 0 | 3.75 | 7.5 | 11.25 | 15 |

# Modeling

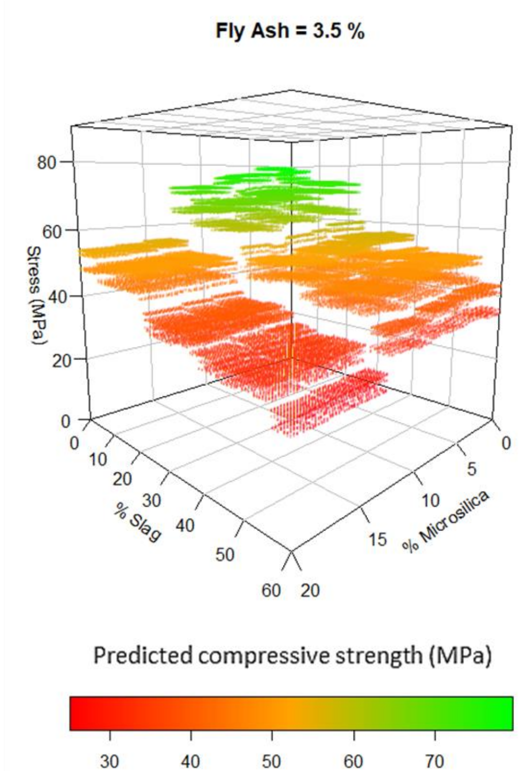
Methods/algorithms:

- kNN
- Random Forest

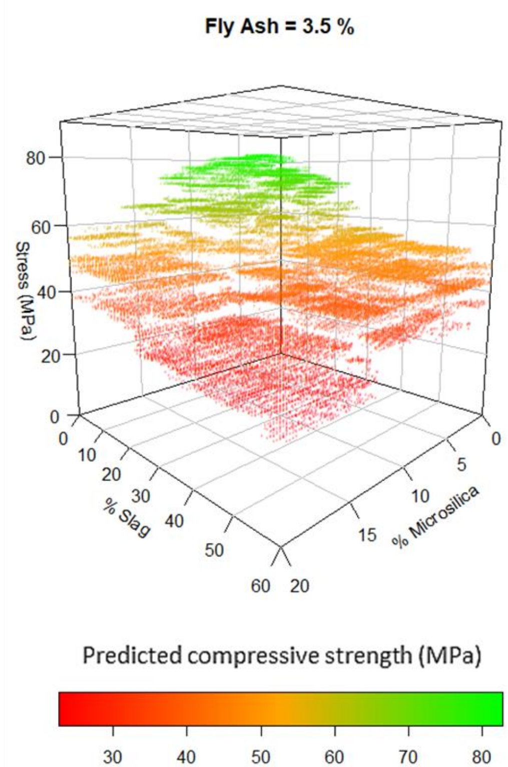
# Modeling




kNN Model




RF Model




Ensemble Model

# Optimization case studies

# Objective

Find optimum binder formulations for:

- *3D printing application*
- *Self-consolidating precast HPC*

# Experimental campaign

Fresh and hardened properties measured:

- *Compressive strength (2h, 4h, 6h, 1d, 7d, 28d)*
- *Static flow (self-consolidating)*
- *Dynamic flow (add energy)*
- *Initial and final setting times*
- *Free shrinkage*

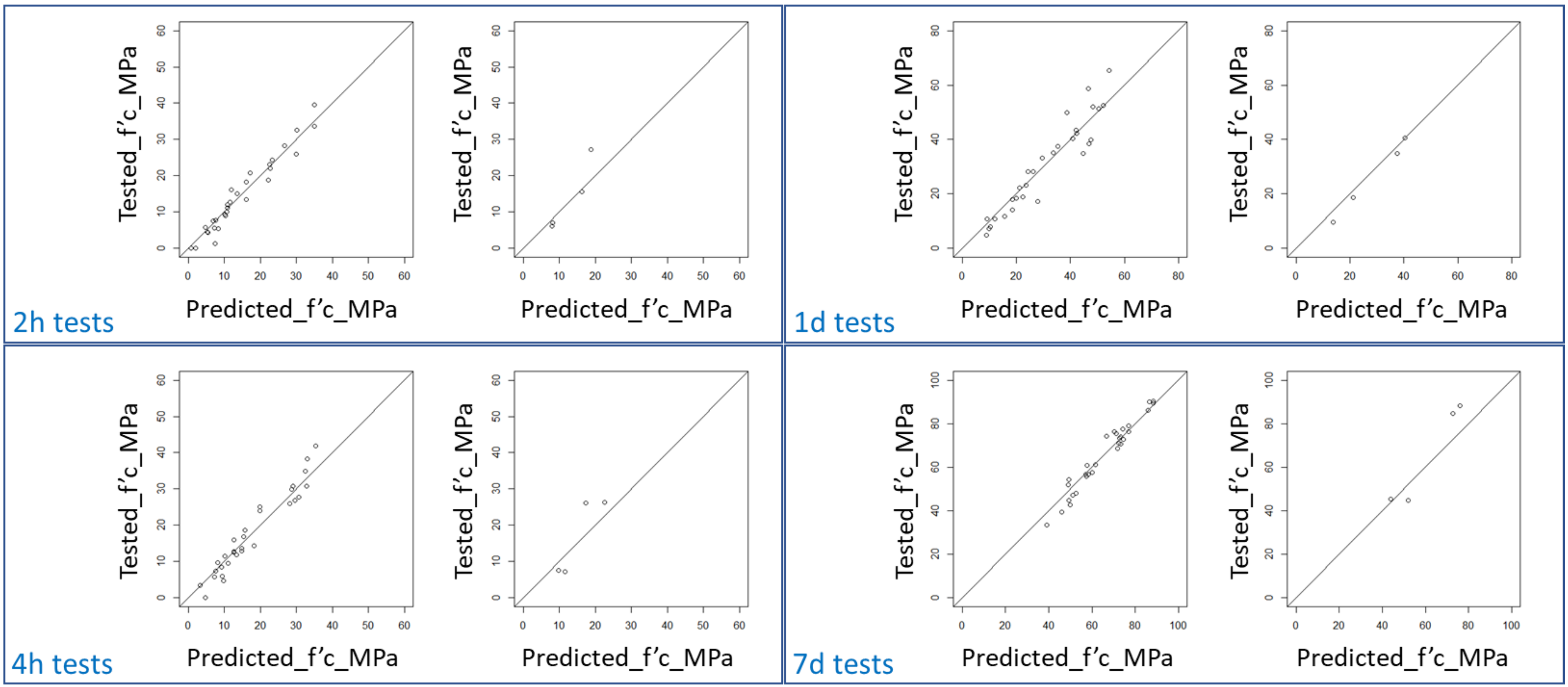
# Design of Experiment (36 mixtures)

Variables:

- *Calcium-aluminate based mineral admixture [10 - 32]%*
- *High-range water reducer to cementitious ratio (HRWR/cm) [0 - 1.25]%*
- *Water-to-cementitious ratio (w/cm) [0.20 - 0.45]*

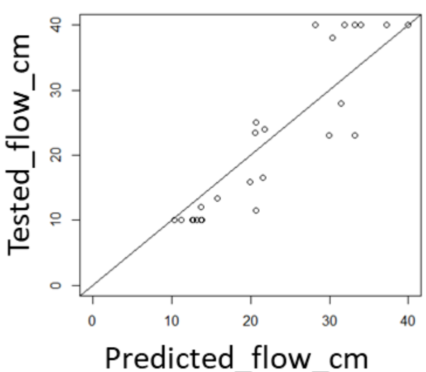
# Estimating compressive strength

TRAIN SET TEST SET TRAIN SET TEST SET

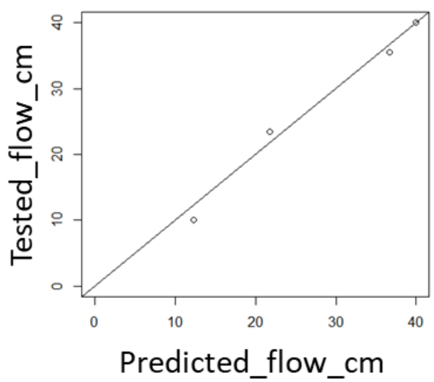


# Estimating static and dynamic flow

TRAIN SET

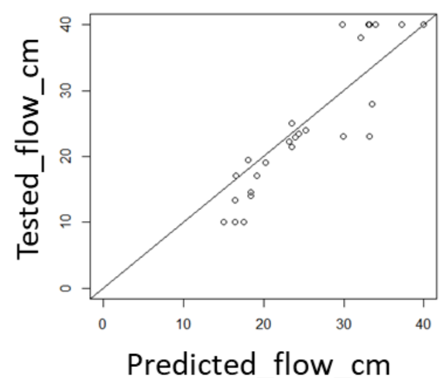



TEST SET

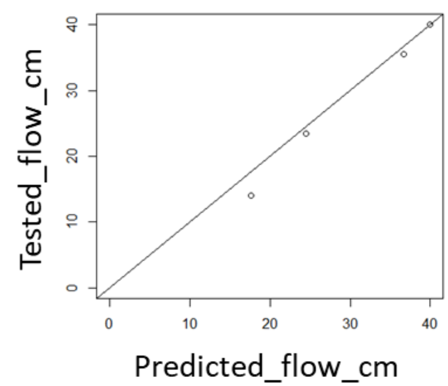



SC_flow

TRAIN SET

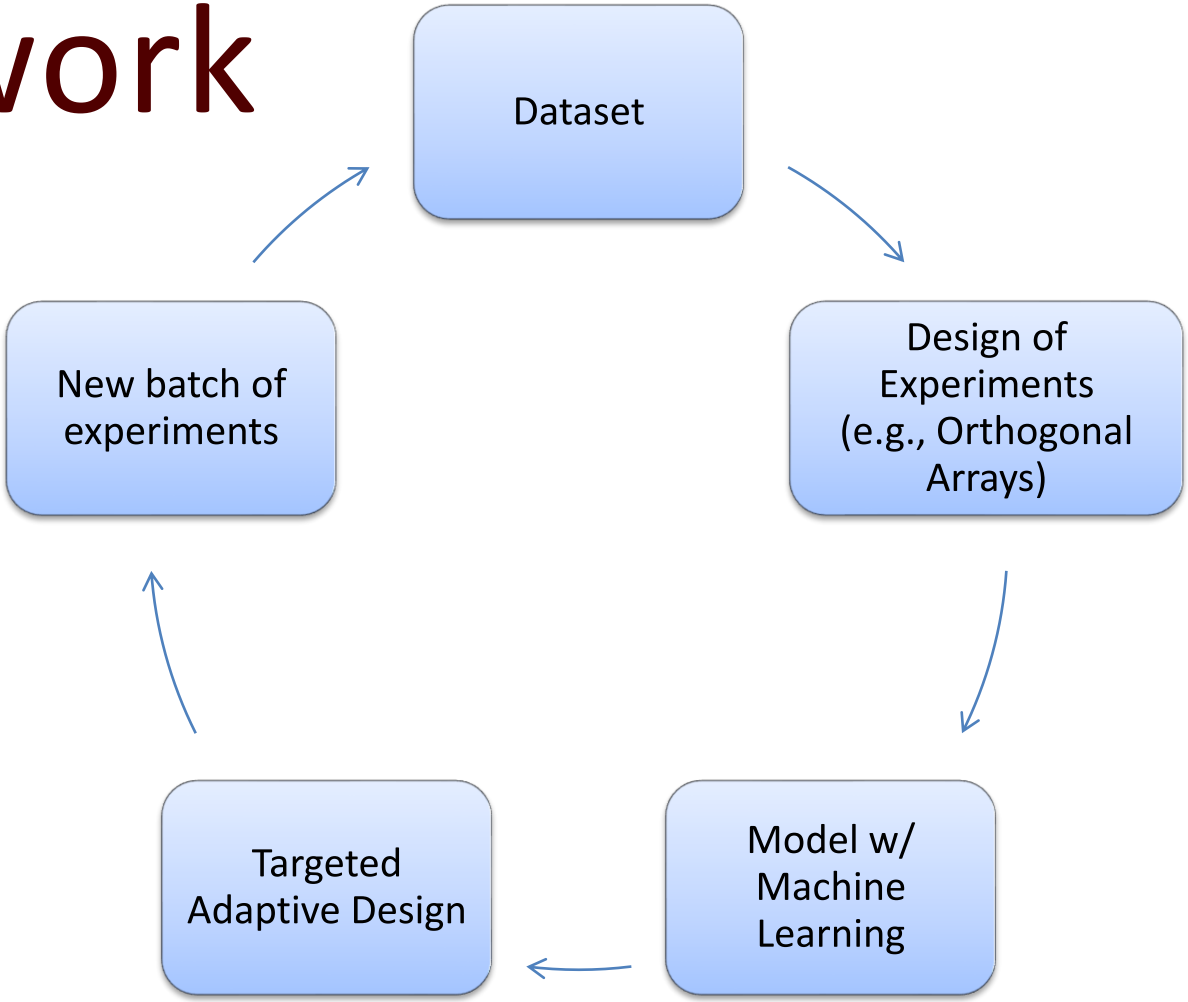



TEST SET




TD_flow

# Future work


Dataset
Design of Experiments (e.g., Orthogonal Arrays)
Model w/ Machine Learning
Targeted Adaptive Design
New batch of experiments

# Key questions addressed in this research

1. Can we effectively optimize concrete mix design w/ **few experimental runs**?

Mixture Design
-> Optimization <-

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***, Cleaner Materials (2022), doi: https://doi.org/10.1016/j.clema.2022.100082

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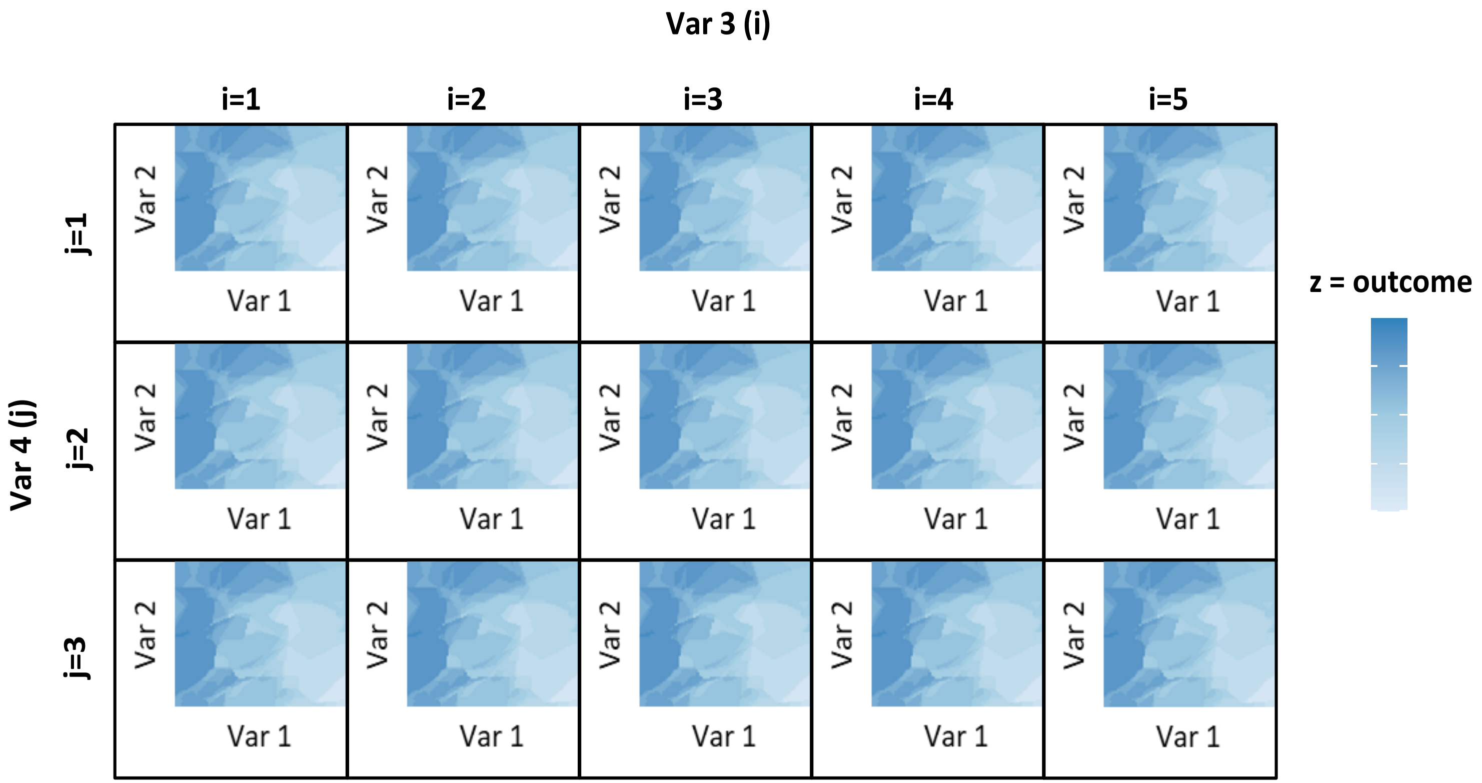
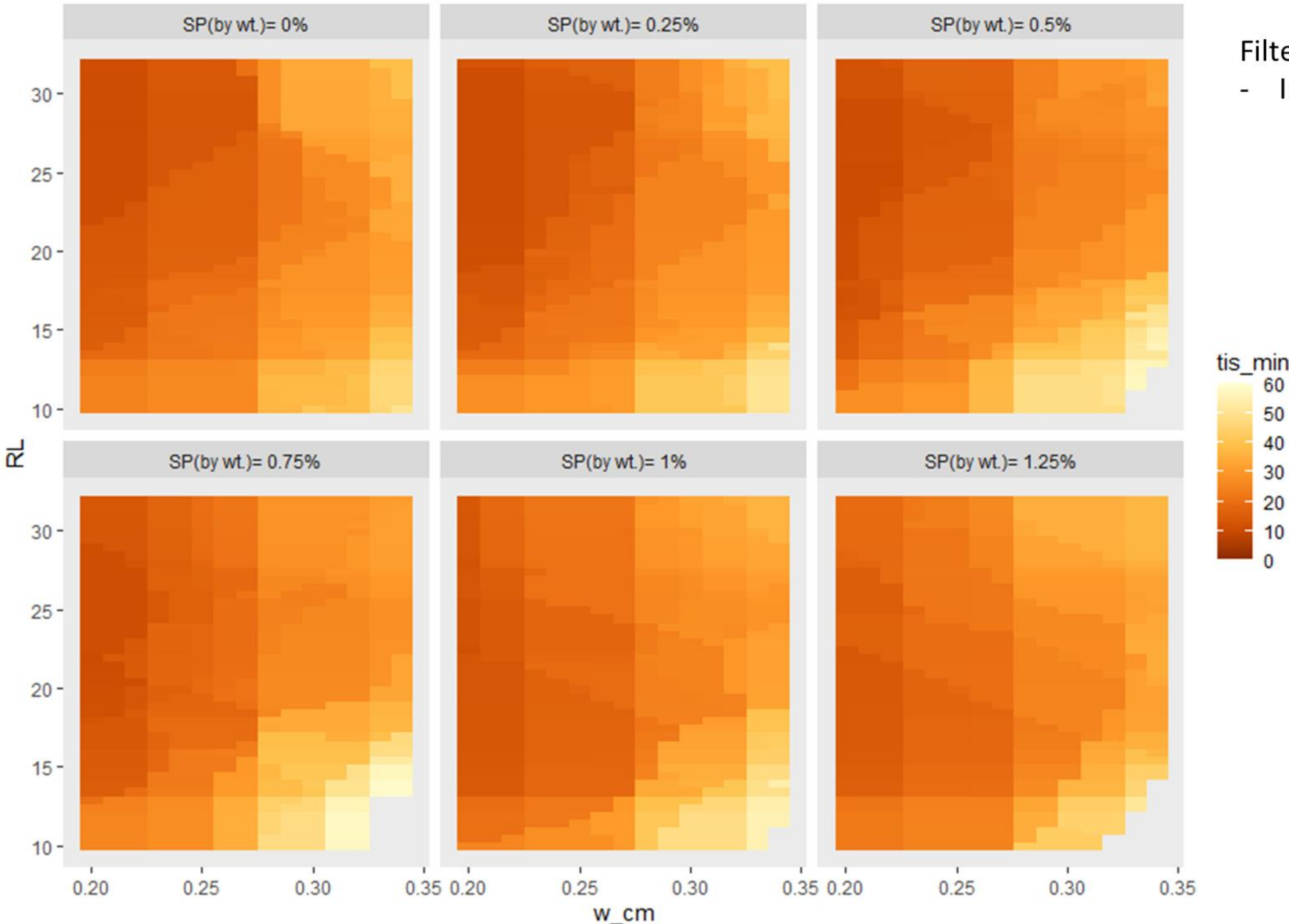
# Performance Density Diagrams

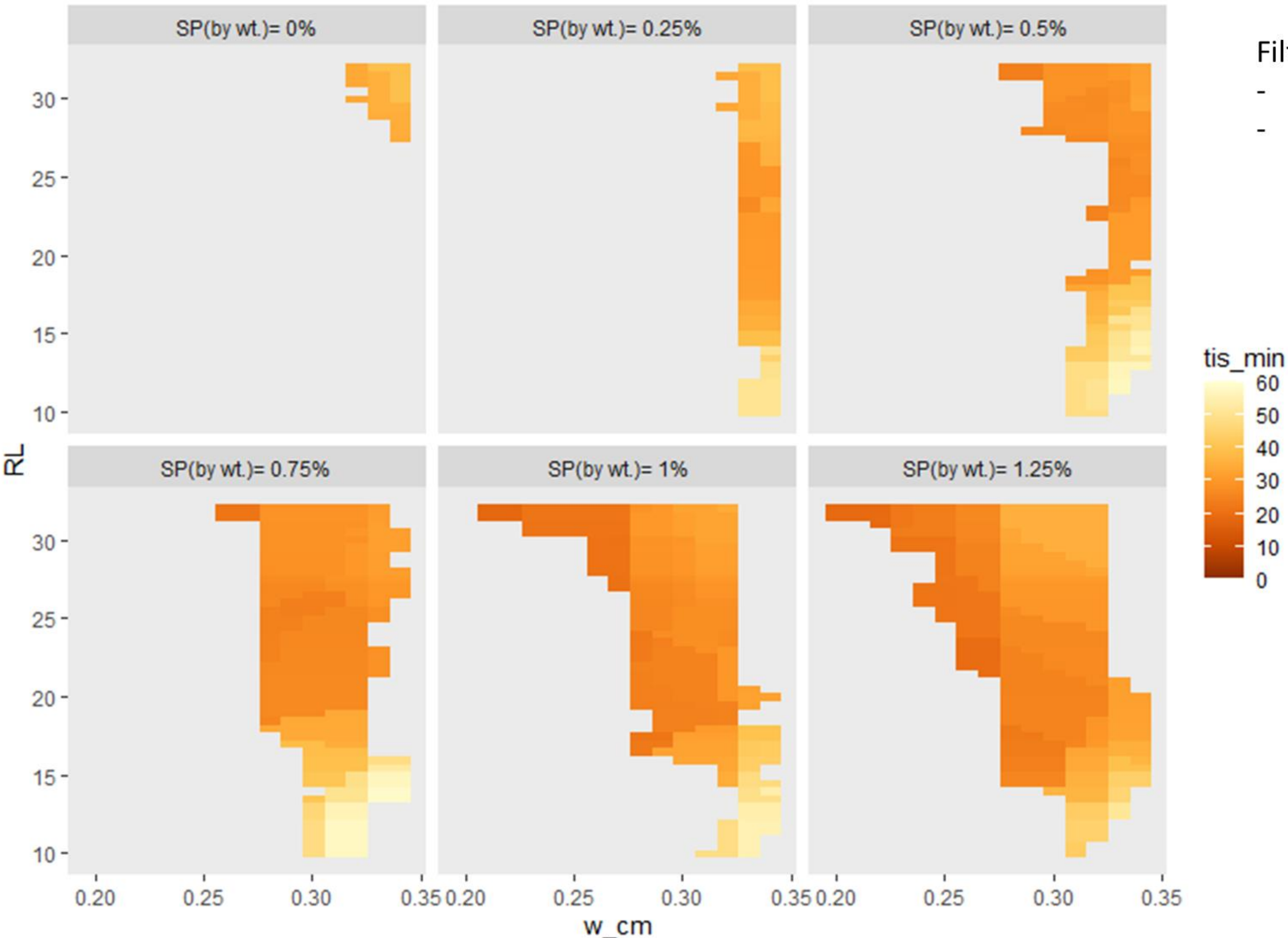
# PDD





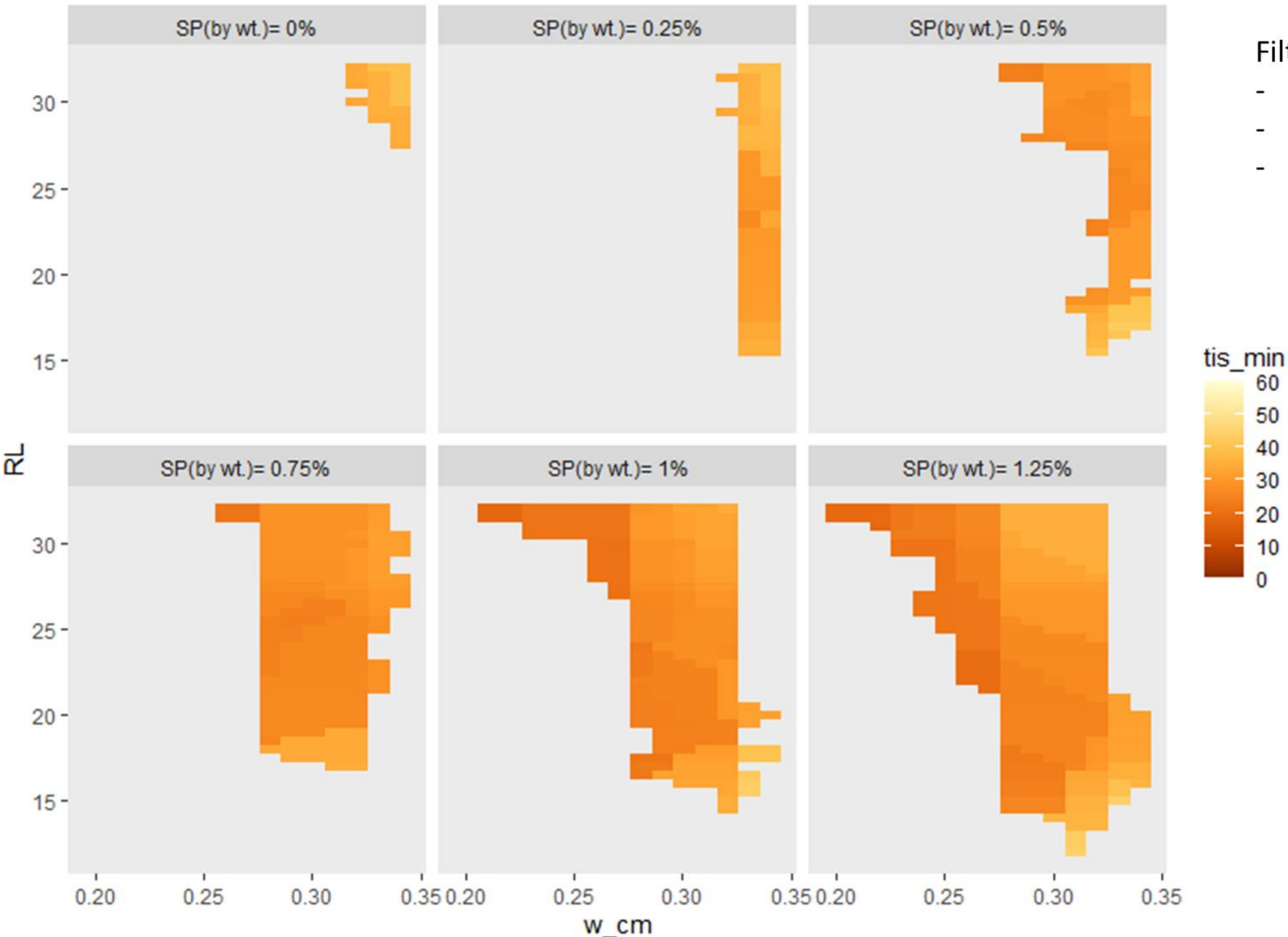

Filters:

- Initial setting time < 60mins



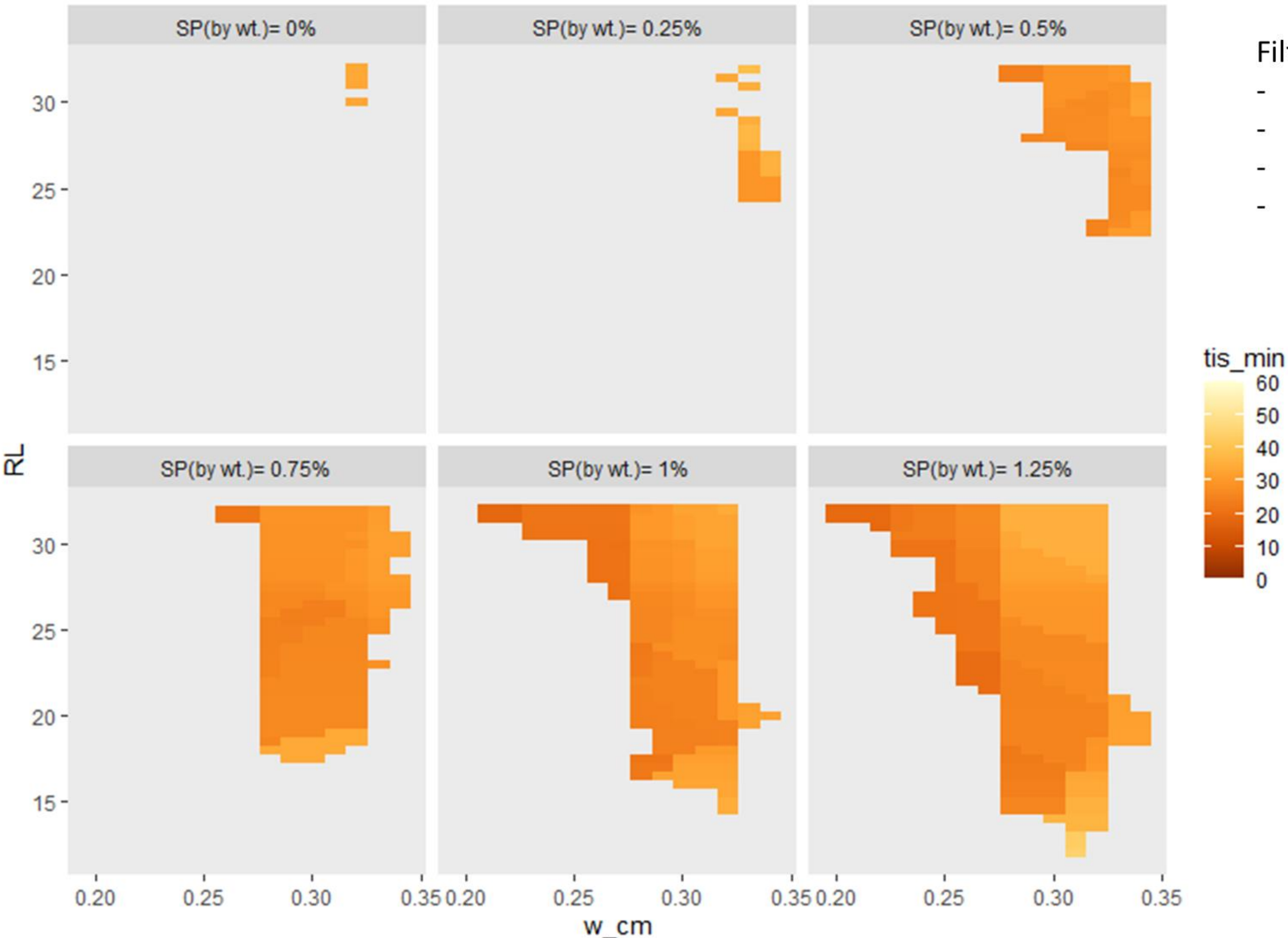

Filters:

- Initial setting time < 60mins
- SC flow = [22-34]cm



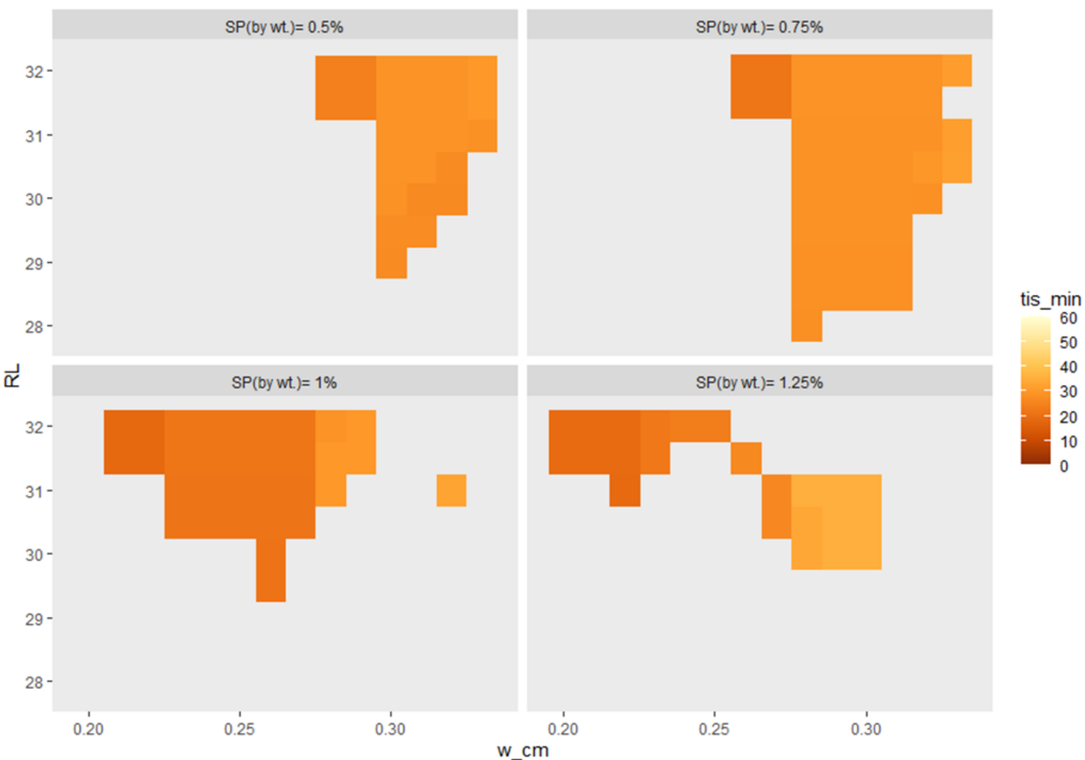

Filters:

- Initial setting time < 60mins
- SC flow = [22-34]cm
- fc_2h > 10 MPa (1450 psi)




Filters:

- Initial setting time < 60mins
- SC flow = [22-34]cm
- fc_2h > 10 MPa (1450 psi)
- fc_6h > 20 MPa (2900 psi)




Filters:

- Initial setting time < 60mins
- SC flow = [22-34]cm
- fc_2h > 10 MPa (1450 psi)
- fc_6h > 20 MPa (2900 psi)
- fc_1d > 30 MPa (4400 psi)
- fc_7d > 50 MPa (7250 psi)
- fc_28d > 60 MPa (8800 psi)
- Free shrinkage < (-1600)με

# *Self-consolidating precast HPC*

**Design Filters:**
- Initial setting time < 60mins
- SC flow = [25-34]cm
- w/cm <0.29
- fc_2h > 22 MPa (3,200 psi)
- fc_4h > 24 MPa (3,500 psi)
- fc_6h > 30 MPa (4,350 psi)
- fc_1d > 44 MPa (6,400 psi)
- fc_7d > 80 MPa (11,600 psi)
- fc_28d > 90 MPa (13,000 psi)

| Mix | RL | w_cm | HRWR_cm |
|---|---|---|---|
| O-SCC-1 | 21 | 0.28 | 1.2 |

Very high risk of cracking

**Design Filters:**
- Initial setting time < 60mins
- SC flow = [25-34]cm
- w/cm <0.27
- fc_2h > 22 MPa (3,200 psi)
- fc_4h > 26 MPa (3,700 psi)
- fc_6h > 28 MPa (4,060 psi)
- fc_1d > 45 MPa (6,525 psi)
- fc_7d > 65 MPa (9,425 psi)
- fc_28d > 70 MPa (10,150 psi)

| Mix | RL | w_cm | HRWR_cm |
|---|---|---|---|
| O-SCC-2 | 30 | 0.26 | 1% |

low risk of cracking

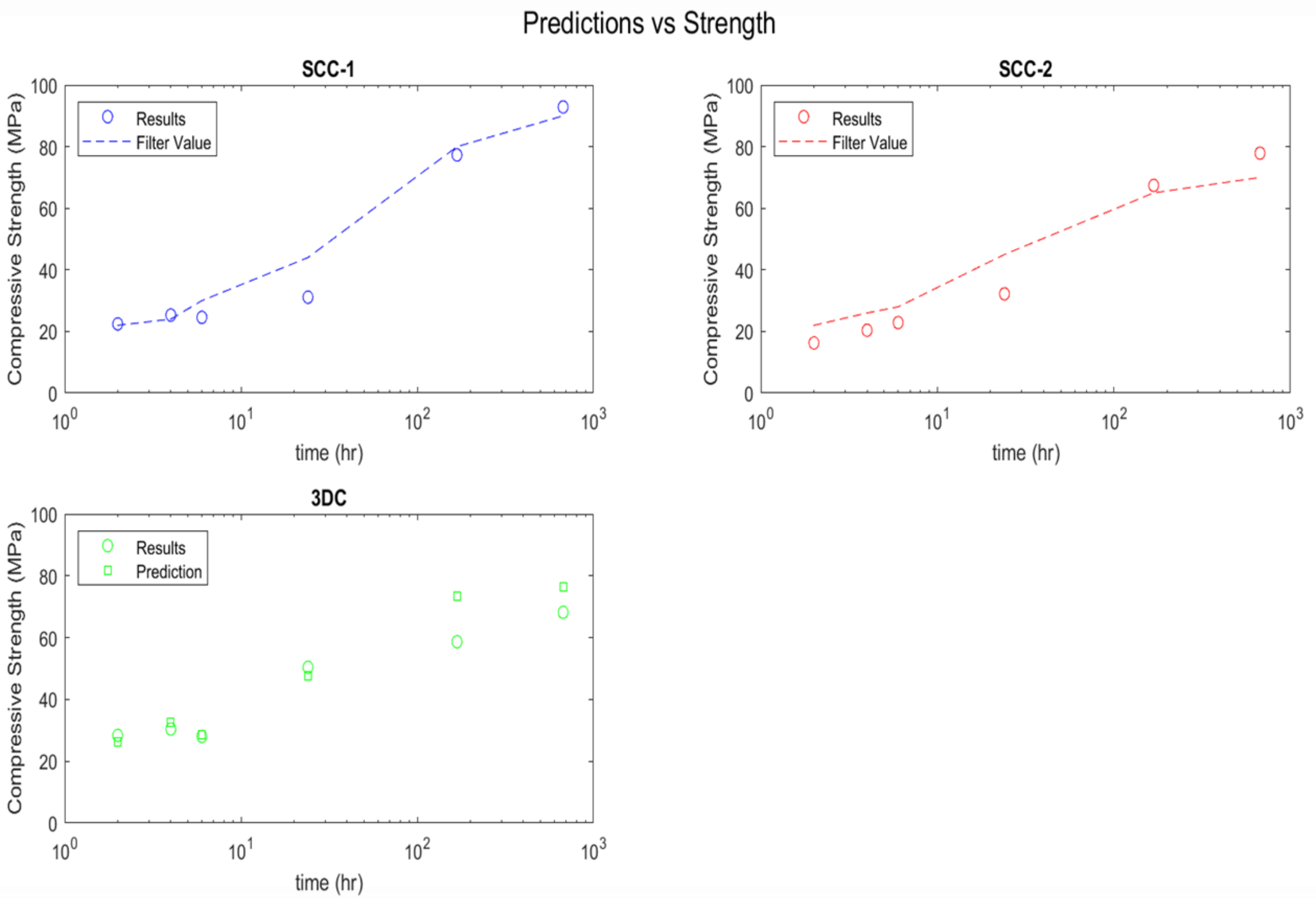
# 3D printing binder

| Mix | RL | w_cm | HRWR_cm |
|---|---|---|---|
| O-3D | 25 | 0.22 | 0.35 |

low risk of cracking

**Design Filters:**

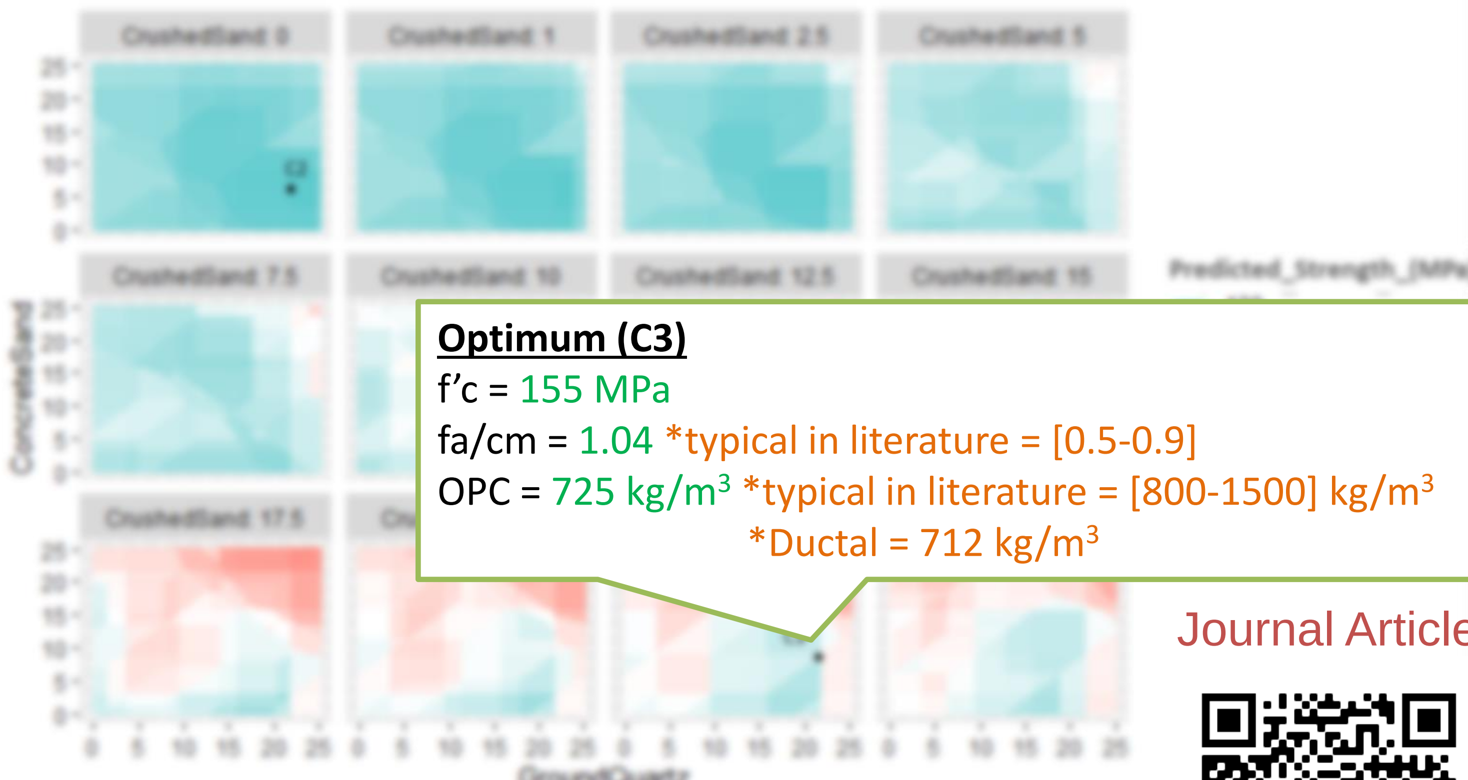
- Initial setting time < 60mins
- HRWR/cm <= 0.5%
- w/cm < 0.26
- RL <= 25%
- SC flow < 11 cm
- TD flow > 13 cm
- fc_2h > 20 MPa (2,900 psi)
- fc_1d > 35 MPa (5,075 psi)



Predictions vs Strength
SCC-1
SCC-2
3DC
Results
Filter Value
Prediction
Compressive Strength (MPa)
time (hr)
0
20
40
60
80
100
$10^0$
$10^1$
$10^2$
$10^3$

# PDD

## UHPC



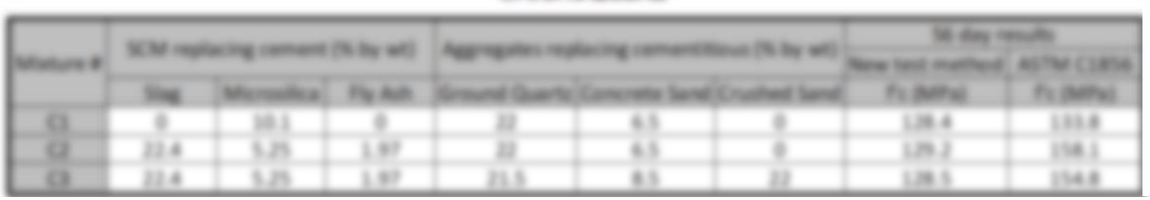
**Optimum (C3)**

f’c = 155 MPa

fa/cm = 1.04 *typical in literature = [0.5-0.9]

OPC = 725 kg/m$^3$ *typical in literature = [800-1500] kg/m$^3$

*Ductal = 712 kg/m$^3$



Journal Article

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1. Can we effectively optimize concrete mix design w/ few experimental runs?

2. Can we evaluate: mechanical performance <- f(changes in mix proportion) in an **easy and intuitive way?**

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

# CONCLUSIONS

1. Can we effectively optimize concrete mix design w/ few experimental runs? -> **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)**

# Related Publications

# Related Publications

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***, Cleaner Materials (2022), doi: https://doi.org/10.1016/j.clema.2022.100082

# Related Publications

**C. Tavares,** Z. Grasley, *Machine Learning-Based Mix Design Tools to Minimize Carbon Footprint and Cost of UHPC.* ***Part 2: Cost- and Eco-Efficiency Density Diagrams***, Cleaner Materials (2022), doi: https://doi.org/10.1016/j.clema.2022.100094

# Related Publications

E Tavares, Cesario Sarmento, Goncalves Martins. (2022). *Multi-objective density diagrams developed with machine learning models to optimize sustainability and cost-efficiency of UHPC mix design* (Order No. 30372235). Available from Dissertations & Theses @ Texas A&M; Dissertations & Theses @ Texas A&M System; ProQuest Dissertations & Theses Global. (2784742994). Retrieved from http://proxy.library.tamu.edu/login?url=https://www.proquest.com/dissertations-theses/multi-objective-density-diagrams-developed-with/docview/2784742994/se-2

# Acknowledgement

*Dr. Skillen's Research Team*

# THANK YOU!

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