# Using the Bulk Oxide Content to Predict Performance of Fly Ash in Concrete with Machine Learning

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# Acknowledgements


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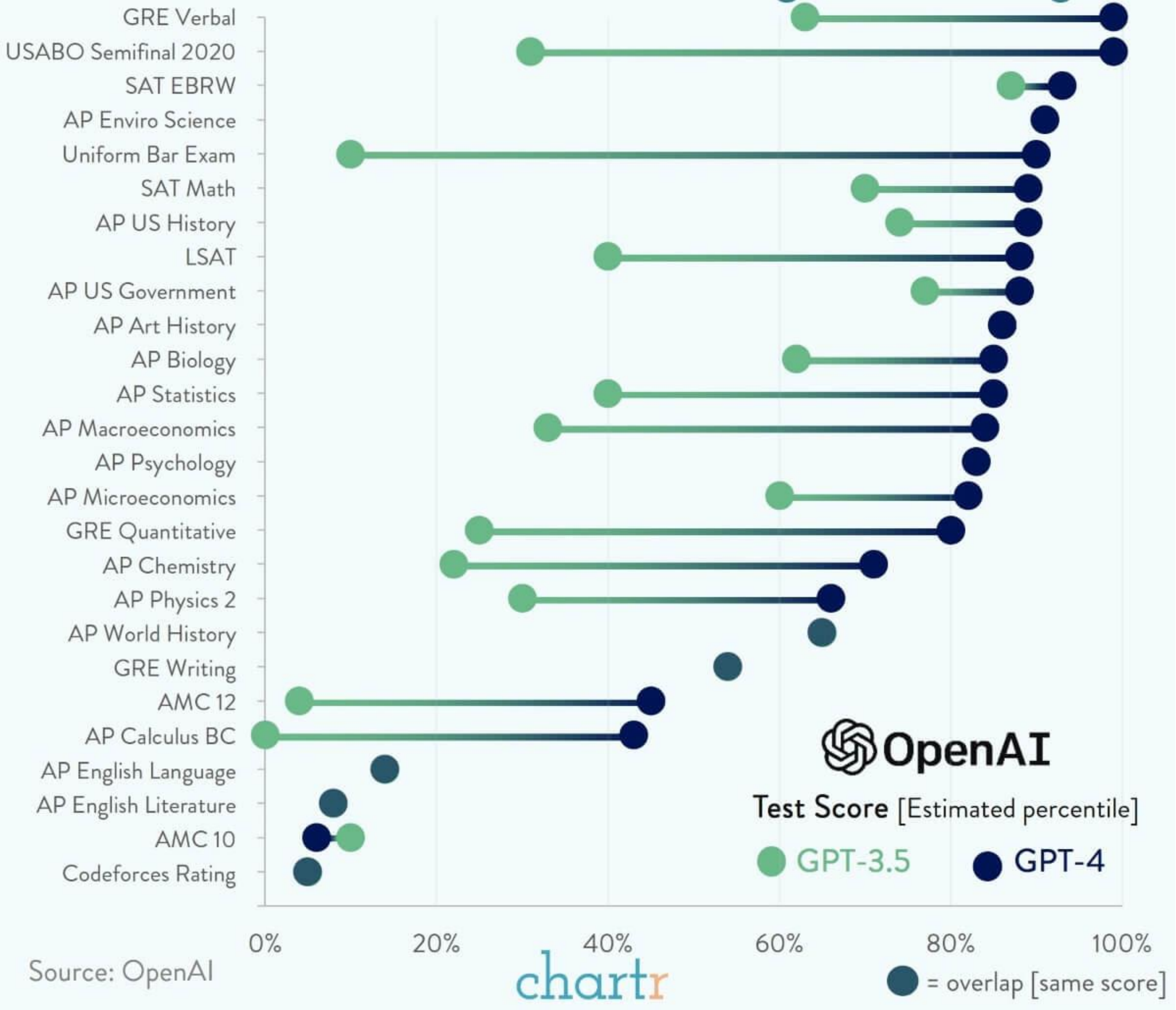
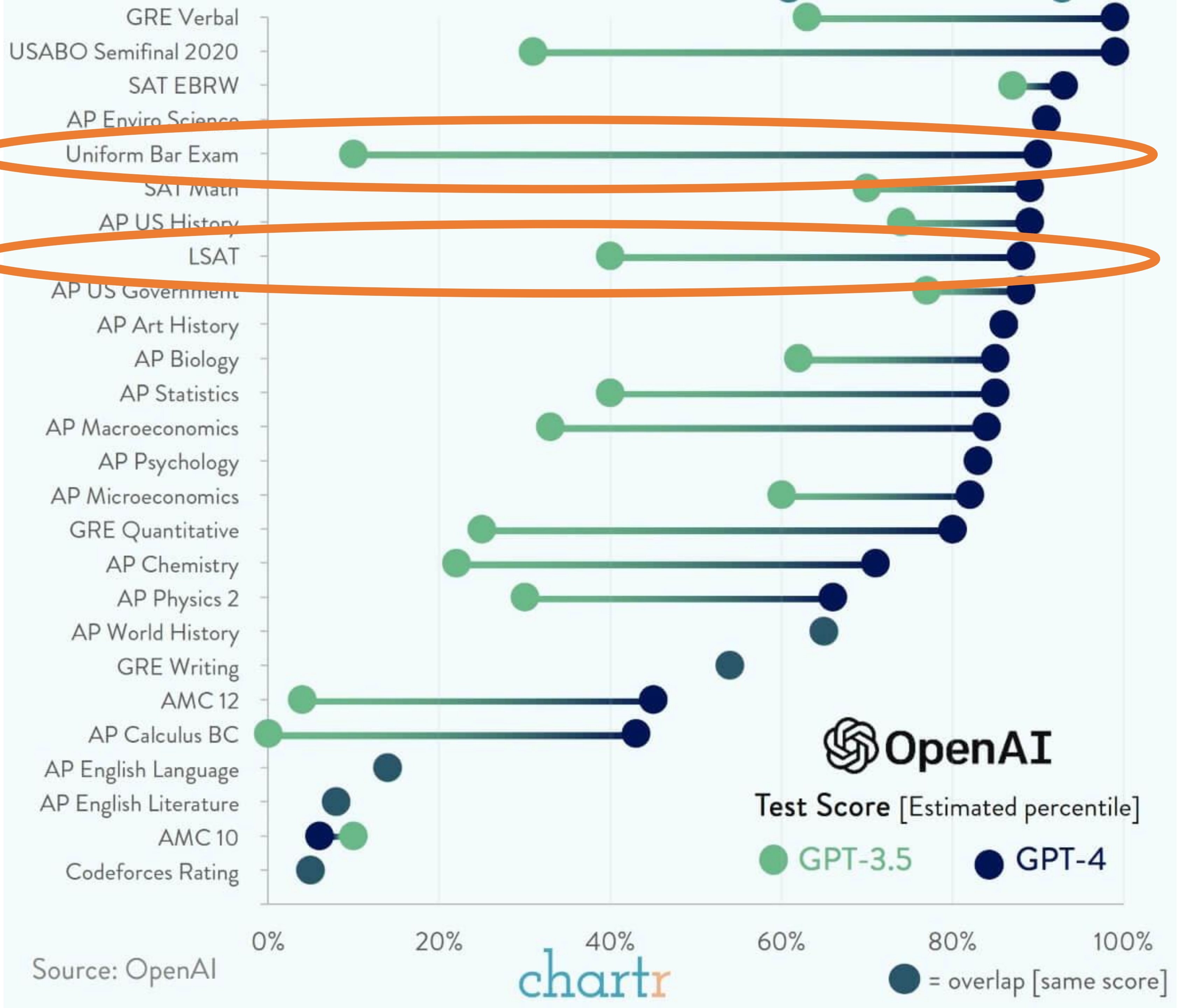
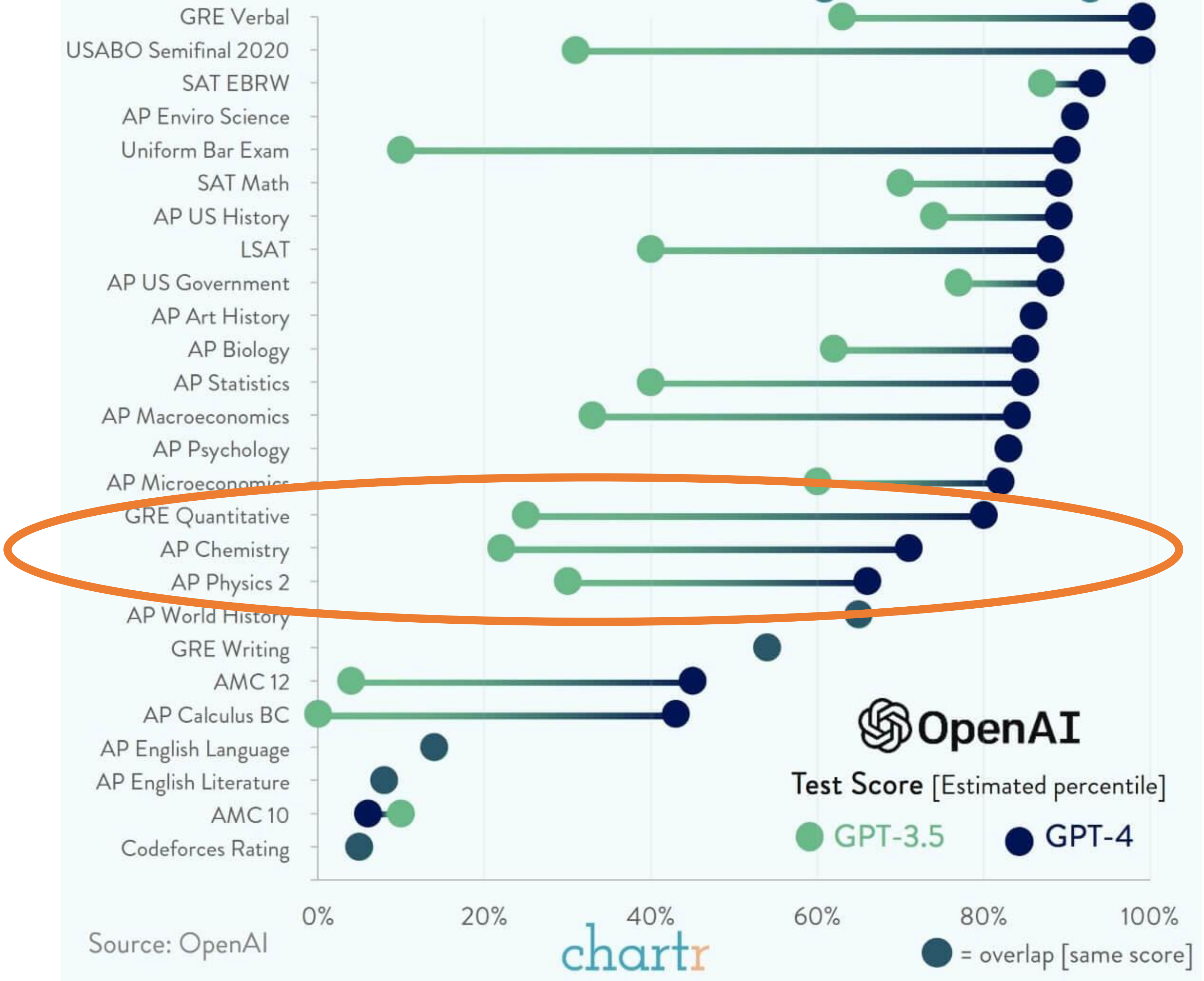
# Will AI and ML change everything?


GRE Verbal
USABO Semifinal 2020
SAT EBRW
AP Enviro Science
Uniform Bar Exam
SAT Math
AP US History
LSAT
AP US Government
AP Art History
AP Biology
AP Statistics
AP Macroeconomics
AP Psychology
AP Microeconomics
GRE Quantitative
AP Chemistry
AP Physics 2
AP World History
GRE Writing
AMC 12
AP Calculus BC
AP English Language
AP English Literature
AMC 10
Codeforces Rating
0%
20%
40%
60%
80%
100%
OpenAI
Test Score [Estimated percentile]
GPT-3.5
GPT-4
= overlap [same score]
Source: OpenAI
chartr




Bar exam

LSAT



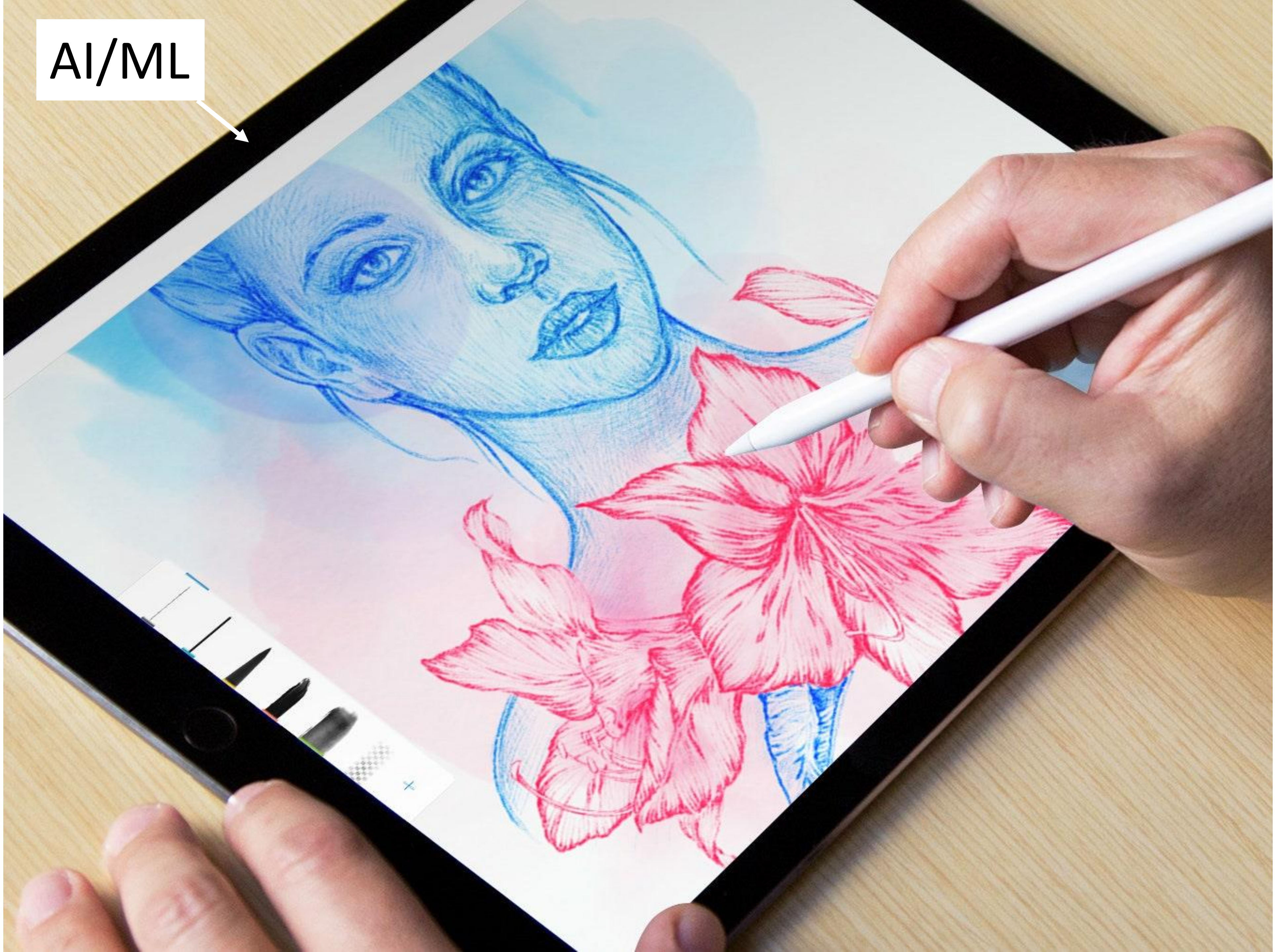

Quantitative tools are improving!

# How do I see AI/ML?


Purdy
Purdy


AI/ML
Purdy
Purdy

AI/ML



# DALL-E 2

```
#generations
curl https://api.openai.com/v1/images/generations \
  -H "Content-Type: application/json" \
  -H "Authorization: Bearer $OPENAI_API_KEY" \
  -d '{
    "prompt": "a photo of a happy corgi puppy sitting and facing forward, stud
    "n":1,
    "size":"1024x1024"
   }'
```

↓

AI/ML

···  Share  Save

“Photograph of llamas in front of the Eiffel tower with sunglasses during the day”

T Tyler × DALL·E
Human & AI

# How do we create **useful** AI/ML tools?

1. Ask a specific and reasonable question
2. Lots of useful data
3. Check the results and improve

# The typical approach

Many AI models try and make precise predictions for a general system.

Unfortunately, you need millions of observations for this, and the results are often not accurate enough.

# A different approach

What if we focused on grouping fly ash performance into high, medium, and low with respect to a control?

This will require less data and can still provide a useful tool.

What if we could do this by only using the bulk oxides?

# Bulk oxides

SGS TEC SERVICES
Testing • Engineering • Consulting

Client: Mr. Tom Hendrix
The SEFA Group
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Moncks Corner, SC 29461

Date: June 24, 2020
TEC Services I.D.: TEC 06-0509
Lab No.: 20-556-MC

**REPORT OF FLY ASH TESTS**

Sample I.D. No.: MC043020 — Date Sampled: April 30, 2020
Manufacturer: McMeekin Station (Thermally Beneficiated) — Date Received: May 6, 2020

| Chemical Analysis | Results (wt%) | Specification (Class F) ASTM C618-19 | Specification (Class F) AASHTO M295-19 |
|---|---|---|---|
| Silicon Dioxide ($SiO_2$) | **54.4** | ---- | ---- |
| Aluminum Oxide ($Al_2O_3$) | **27.2** | ---- | ---- |
| Iron Oxide ($Fe_2O_3$) | **6.82** | ---- | ---- |
| Sum of Silicon Dioxide, Iron Oxide & Aluminum Oxide ($SiO_2+Al_2O_3+Fe_2O_3$) | **88.4** | 50.0 % min. | 50.0 % min. |
| Calcium Oxide (CaO) | **2.4** | 18.0 % max. | 18.0 % max. |
| Magnesium Oxide (MgO) | **1.1** | ---- | ---- |
| Sodium Oxide ($Na_2O$) | **0.29** | ---- | ---- |
| Potassium Oxide ($K_2O$) | **2.52** | ---- | ---- |
| "Sodium Oxide Equivalent ($Na_2O+0.658K_2O$)" | **1.95** | ---- | ---- |
| Sulfur Trioxide ($SO_3$) | **0.09** | 5.0 % max. | 5.0 % max. |
| Loss on Ignition | **0.5** | 6.0 % max. | 5.0 % max. |
| Moisture Content | **0.1** | 3.0 % max. | 3.0 % max. |
| **Available Alkalies** | | | |
| Sodium Oxide ($Na_2O$) as Available Alkalies | **0.10** | ---- | ---- |
| Potassium Oxide ($K_2O$) as Available Alkalies | **1.04** | ---- | ---- |
| Available Alkalies as "Sodium Oxide Equivalent ($Na_2O+0.658K_2O$)" | **0.78** | ---- | 1.5 % max.* |

| Physical Analysis | Test Date | Result | ASTM C618-19 | AASHTO M295-19 |
|---|---|---|---|---|
| Fineness (Amount Retained on #325 Sieve) | 5/13/20 | **16.1%** | 34 % max. | 34 % max. |
| Strength Activity Index (Using Lehigh Leeds Alabama Portland Cement) | | | | |
| At 7 Days: Control Average, psi: 4690; Test Average, psi: 3940 | 5/26/20 | **84%** | 75 % min.† (of control) | 75 % min.† (of control) |
| At 28 Days: Control Average, psi: 5870; Test Average, psi: 5560 | 6/16/20 | **95%** | 75 % min.† (of control) | 75 % min.† (of control) |
| Water Requirements (Test $H_2O$/Control $H_2O$) Control, mls: 242; Test, mls: 234 | 5/19/20 | **97%** | 105% max.† (of control) | 105% max.† (of control) |
| Autoclave Expansion: | 5/13/20 | **-0.04%** | ± 0.8 % max. | ± 0.8 % max. |

| Uniformity Requirements | | | | Test Date | Variation | ASTM C618-19 | AASHTO M295-19 |
|---|---|---|---|---|---|---|---|
| Specific Gravity: | **2.32** | Average: | **2.33** | 5/13/20 | **-0.4%** | 5 % max. from average | 5 % max. from average |
| % Retained #325 Sieve: | **16.1** | Average: | **14.2** | 5/13/20 | **1.9%** | 5 % max. from average | 5 % max. from average |

† Meeting the 7 day or 28 day strength activity index will indicate specification compliance
* Optional
**Chemical Analysis performed on May 20, 2020.

The results of our testing indicate that this sample complies with ASTM C618-19 and AASHTO M295-19 specifications for Class F pozzolans.

Respectfully Submitted,
**SGS TEC Services**

Dean Roosa
Project Manager

Shawn McCormick
Laboratory Principal

ISO 17025 ACCREDITED LABORATORY — US Army Corps of Engineers — AASHTO R18 — ASTM INTERNATIONAL

SGS TEC SERVICES
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| | Mass % |
|---|---|
| $SiO_2$ | 36.2 |
| $Al_2O_3$ | 21.7 |
| $Fe_2O_3$ | 5.3 |
| CaO | 23.1 |
| MgO | 5.3 |
| $SO_3$ | 0.6 |
| $Na_2O$ | 3.5 |
| $K_2O$ | 1.0 |
| $TiO_2$ | 0.8 |
| $P_2O_5$ | 1.9 |
| SrO | 0.2 |

# Classification Steps

How does a concrete mixture with fly ash compare to a mixture with only portland cement?

Create performance classes

- Class 1: < portland cement mean – 1 std
- Class 2: = portland cement mean +/- 1 std
- Class 3: > portland cement + 1 std

# Classification Steps

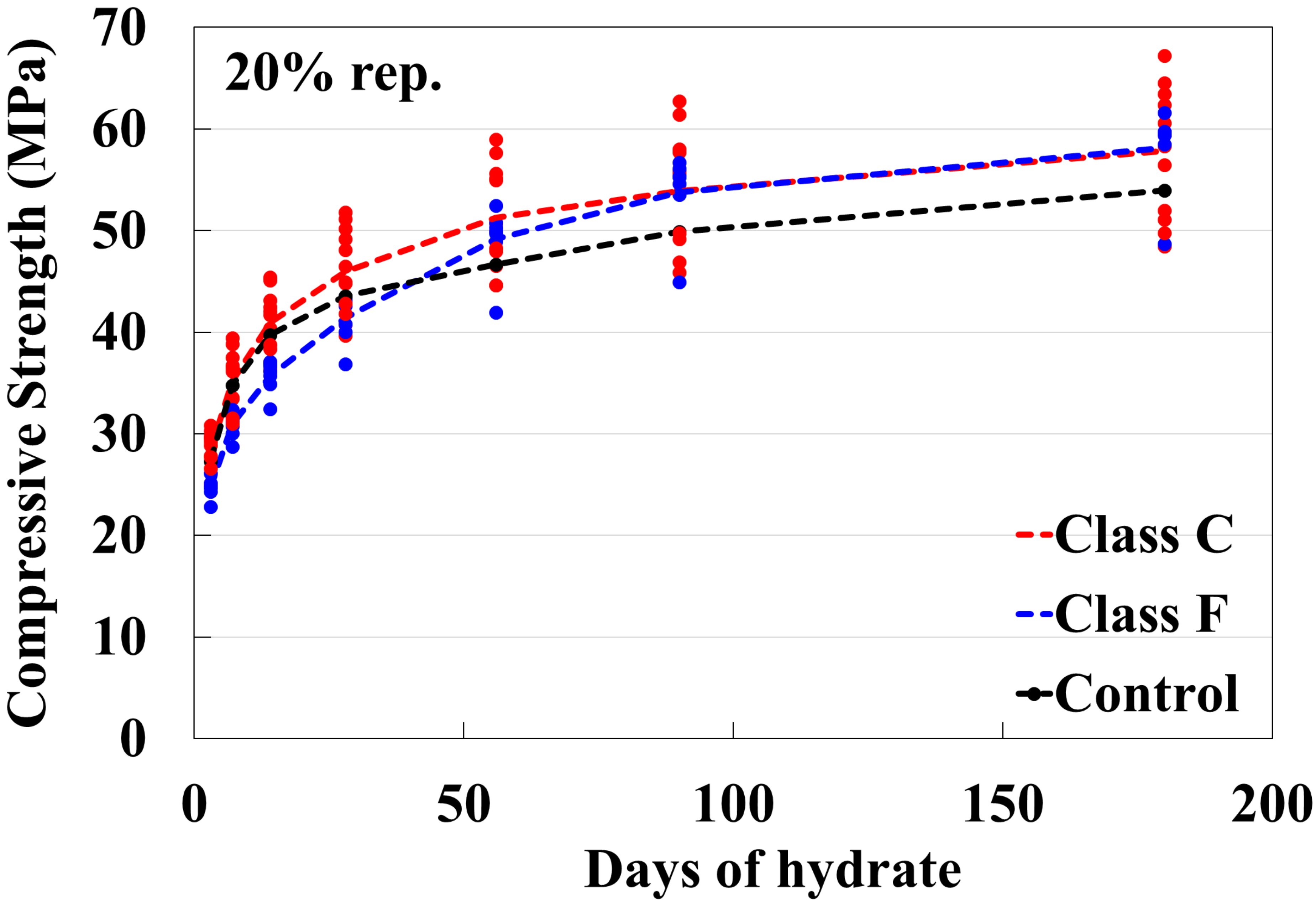
How does a concrete mixture with fly ash compare to a mixture with only portland cement?

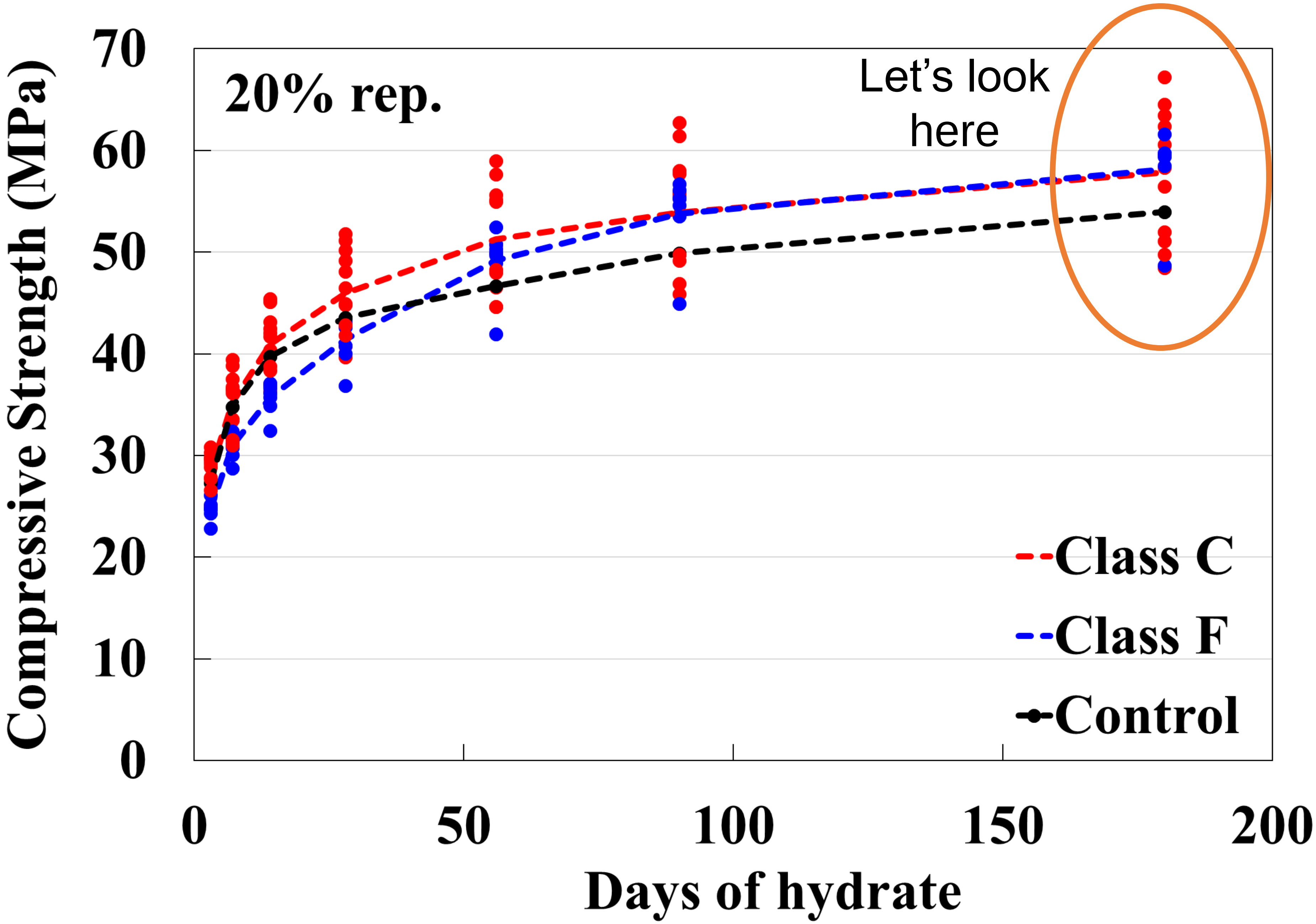
Create performance classes

Class 1: < OPC – 1 std

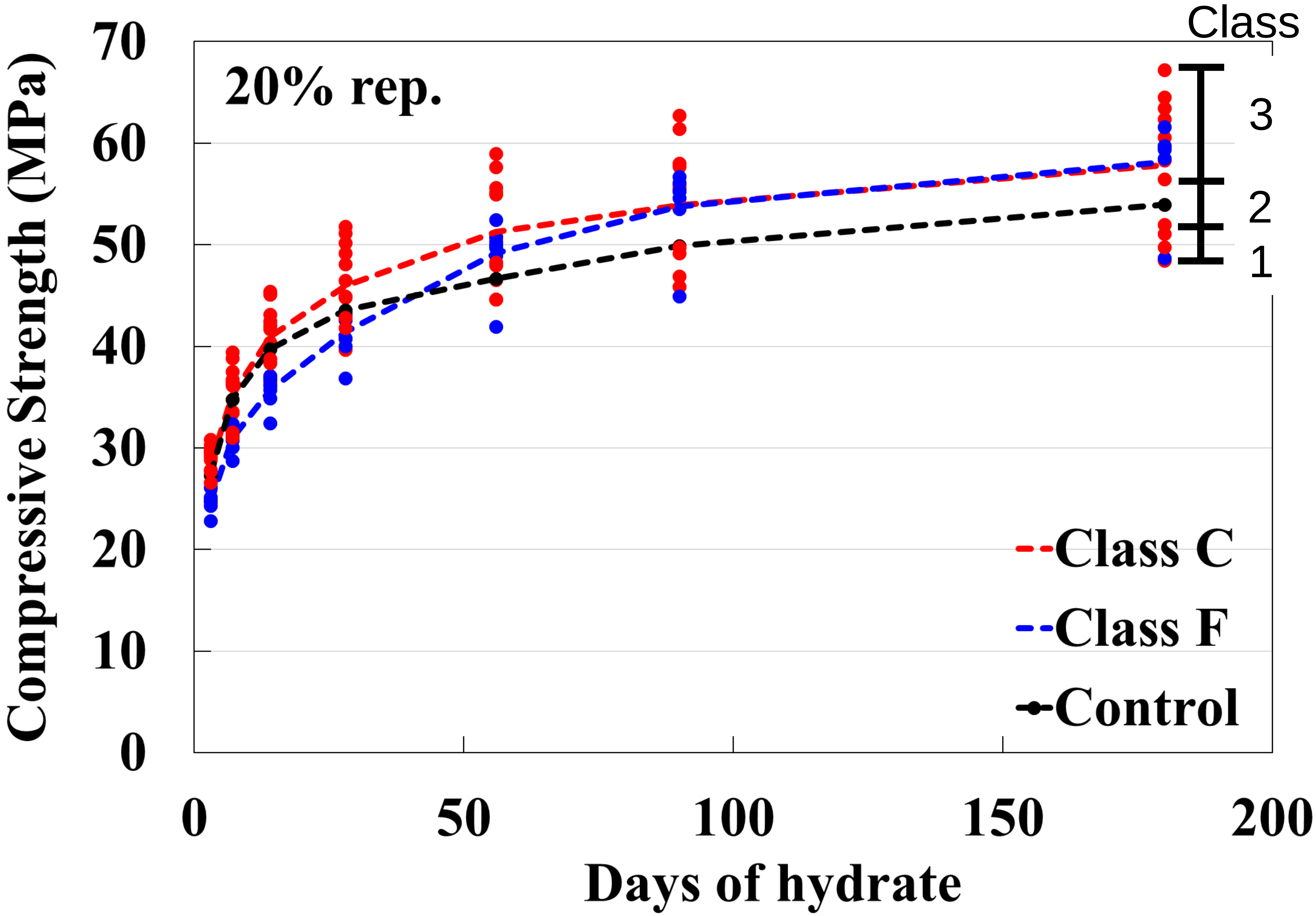
Class 2: Same as OPC +/- 1 std

Class 3: > OPC


20% rep.
Compressive Strength (MPa)
70
60
50
40
30
20
10
0
0
50
100
150
200
Days of hydrate
Class C
Class F
Control



Compressive Strength (MPa)
70
60
50
40
30
20
10
0
20% rep.
Let's look here
Class C
Class F
Control
0
50
100
150
200
Days of hydrate



Class
20% rep.
3
2
1
Compressive Strength (MPa)
0
10
20
30
40
50
60
70
0
50
100
150
200
Days of hydrate
Class C
Class F
Control

# Data

30 traditional + 14 harvested fly ashes

22 Class C

22 Class F

Tested at 20% and 40% replacement

Compare performance with a standard concrete mixture

# Data

0.45 w/cm, 6.6 sacks of binder, Type I cement, one coarse and fine aggregate source.

| | |
|---|---|
| Compression Strength | 3, 7, 14, 28, 56, 90, 180d |
| Resistivity | 3, 7, 14, 28, 56, 90, 180d |
| Diffusion Coefficient | 35, 70, 135, 200, 500, 700d |
| Heat of Hydration | 48h |

# Data

0.45 w/cm, 6.6 sacks of binder, Type I cement, one coarse and fine aggregate source.

**2655 measurements**

| | |
|---|---|
| Diffusion Coefficient | 35, 70, 135, 200, 500, 700d |
| Heat of Hydration | 48h |

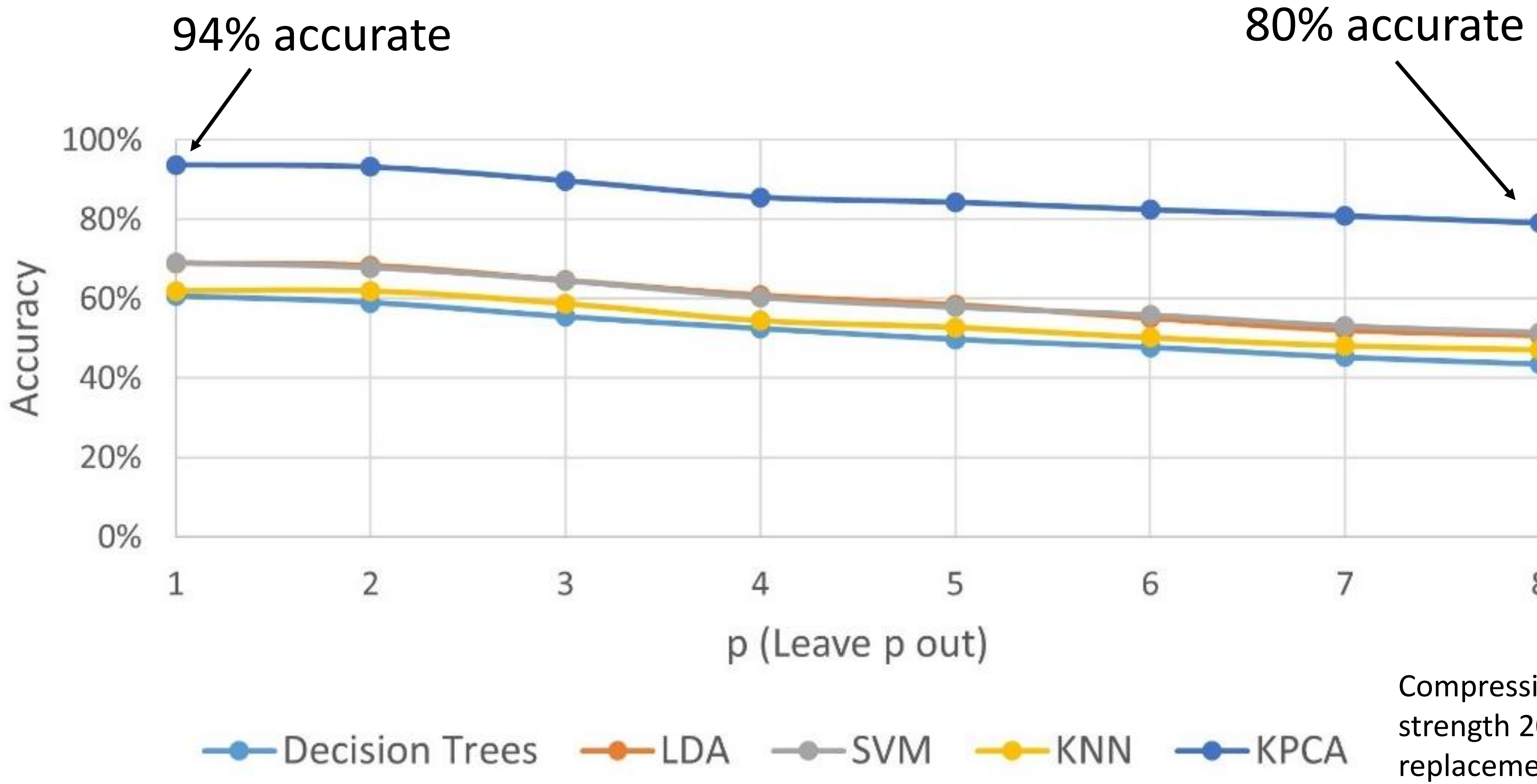
# Classification Steps

Compared 5 ML models that use all 11 bulk oxides.

Rank the models by using
Leave Out X Cross Validation (LOXCV)

For x = 1 - Use 43 (44-1) observations as the training set and the remaining observation to check.

Repeat this 43 times and report the % accuracy




Compressive strength 20% replacement all time periods.

The best model is Kernel Principal Component Analysis (Kernel PCA)

We call it Kermit PCA

Is the mixture?

Class 1: < OPC
Class 2: Same as OPC
Class 3: > OPC

# Compressive strength

| Days of hydration | 20% replacement | 40% replacement |
|---|---|---|
| 3d | 98% | 100% |
| 7d | 93% | 91% |
| 14d | 98% | 91% |
| 28d | 95% | 85% |
| 56d | 93% | 82% |
| 90d | 91% | 79% |
| 180d | 89% | 81% |
| AVG | 94% | 87% |

Accuracy

Is the mixture?

Class 1: < OPC
Class 2: Same as OPC
Class 3: > OPC

## Diffusion Coefficient

| **Days of hydration** | **20% replacement** | **40% replacement** |
|---|---|---|
| 45d | 83% | 83% |
| 90d | 72% | 76% |
| 135d | 83% | 72% |
| 200d | 76% | 76% |
| 250d | 76% | 82% |
| 500d | 82% | 76% |
| 700d | 76% | 78% |
| AVG | 79% | 78% |

Accuracy

Is the mixture?

Class 1: < OPC
Class 2: Same as OPC
Class 3: > OPC

# Heat of Hydration

| Hours of hydration | 20% replacement | 40% replacement |
|---|---|---|
| 48h | 83% | 77% |

Accuracy

# Discussion

The Kermit PCA analysis is able to use the bulk oxides to group the performance of the fly ash and harvested fly ash for 20% and 40% replacement with 44 ashes for strength, diffusion, heat, and diffusion with about 85% (94% to 77%) accuracy.

This can be a powerful tool!!!

# How can you implement?

Input bulk oxides into a simple web interface.

Website will do the calculations and tell you how it will perform compared to OPC.

www.tylerley.com/flyash

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# Fly Ash Performance Calculator

| Chemical Components (by mass %) | |
|---|---|
| $SiO_2$ | 36.2 |
| $Al_2O_3$ | 21.7 |
| $Fe_2O_3$ | 5.35 |
| CaO | 23.15 |
| MgO | 5.38 |
| $SO_3$ | .67 |
| $Na_2O$ | 3.58 |
| $K_2O$ | 1 |
| $TiO_2$ | .8 |
| $P_2O_5$ | 1.9 |
| SrO | .23 |
| Total | 99.96 |

Calculate

| Compressive Strength | | |
|---|---|---|
| Fly Ash Replacement by Mass | 20% | 40% |
| 3d | Same | Lower |
| 7d | Same | Same |
| 14d | Same | Higher |
| 28d | Higher | Higher |
| 56d | Higher | Higher |
| 90d | Higher | Higher |
| 180d | Higher | Higher |

| Diffusion Coefficient | | |
|---|---|---|
| Fly Ash Replacement by Mass | 20% | 40% |
| 45d | Same | Lower |
| 90d | Same | Lower |
| 135d | Same | Lower |

Lower = lower than a mixture with just OPC
Same = same as a mixture with just OPC
Higher = higher than a mixture with just OPC

# How could this be used?

Rapid screening tool to understand how a fly ash source will impact your mixture design

Investigating blends of fly ash

Investigating fly ash that does not meet current specs

Build confidence in harvested fly ash

# What would you do with this info?

This provides deeper insights besides Class C and F.

We are about to enter a new era of fly ash and we need all the help we can get.

# Why does this work?

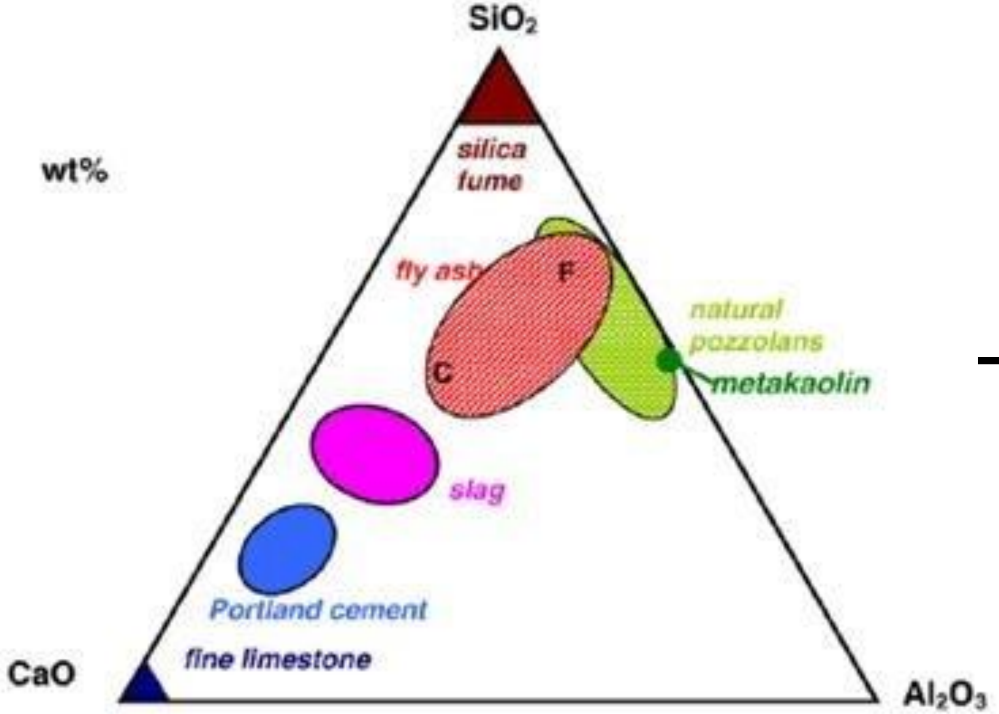
Particle size distribution is similar between these ashes

We have always known that chemical composition is important

Class C $\geq$ 18% CaO

Class F $<$ 18% CaO

Now we can take into account all the oxides.


SiO2
wt%
silica fume
fly ash
F
C
natural pozzolans
metakaolin
slag
Portland cement
fine limestone
CaO
Al2O3

# What is next?

Finish ASR model for ASTM C 1567

Use 20 independent fly ashes to validate results

Investigate cements with different alkalis

A method that uses tables to do the same thing.  This could be used in a guide document.

# Conclusion

ML tools are powerful and will help us develop new understanding and insights into some long standing questions.

The Kermit PCA model is able accurately predict the performance of both traditional and harvested fly ash for compressive strength, resistivity, diffusion, and heat of hydration.

www.tylerley.com/flyash

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# Fly Ash Performance Calculator

| Chemical Components (by mass %) | |
|---|---|
| $SiO_2$ | 36.2 |
| $Al_2O_3$ | 21.7 |
| $Fe_2O_3$ | 5.35 |
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| MgO | 5.38 |
| $SO_3$ | .67 |
| $Na_2O$ | 3.58 |
| $K_2O$ | 1 |
| $TiO_2$ | .8 |
| $P_2O_5$ | 1.9 |
| SrO | .23 |
| Total | 99.96 |

Calculate

| Compressive Strength | | |
|---|---|---|
| Fly Ash Replacement by Mass | 20% | 40% |
| 3d | Same | Lower |
| 7d | Same | Same |
| 14d | Same | Higher |
| 28d | Higher | Higher |
| 56d | Higher | Higher |
| 90d | Higher | Higher |
| 180d | Higher | Higher |

| Diffusion Coefficient | | |
|---|---|---|
| Fly Ash Replacement by Mass | 20% | 40% |
| 45d | Same | Lower |
| 90d | Same | Lower |
| 135d | Same | Lower |

Lower = lower than a mixture with just OPC
Same = same as a mixture with just OPC
Higher = higher than a mixture with just OPC

www.tylerley.com/flyash
www.youtube.com/tylerley
tyler.ley@okstate.edu

| Mixture | w/cm | Cement (lbs) | Fly Ash (lbs) | Water (lbs) | Paste (%) | Coarse (lbs) | Fine (lbs) |
|---|---|---|---|---|---|---|---|
| 100% OPC | 0.45 | 625 | 0 | 281 | 28.8 | 1903 | 1243 |
| 20% Fly Ash | 0.45 | 500 | 125 | 281 | 28.9 | 1900 | 1240 |
| 40% Fly Ash | 0.45 | 375 | 250 | 281 | 29.0 | 1892 | 1228 |

Is the mixture?

Class 1: < OPC
Class 2: Same as OPC
Class 3: > OPC

## Resistivity

| Days of hydration | 20% replacement | 40% replacement |
|---|---|---|
| 3d | 73% | 79% |
| 7d | 81% | 68% |
| 14d | 66% | 67% |
| 28d | 69% | 91% |
| 56d | 86% | 79% |
| 90d | 81% | 71% |
| 180d | 82% | 85% |
| AVG | 77% | 77% |

Accuracy