

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



Tyler Ley, PE, PhD

Shinhyu Kang, Taehwan Kim, Braden Boyd,
Zane Lloyd, Niloo Parastegari, Zhe Yu, Guoliang Fan

Acknowledgements

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Cecil Jones, Diversified Engineering

Thoughts on Computational Tools

Thoughts on Computational Tools

All computational models are wrong,
but they can give us insights that are
not possible any other way.

- Zach Grasley



Thoughts on Computational Tools

Computational models that are based on the truth are powerful, but we need experiments to tell us the truth.

- Tyler Ley



Different types of models

- Statistical models
- Physics based
- AI/ML

How do we create useful computational tools?

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


Physics based model

- Pick a reasonable model with adjustable parameters
- Gather data
- Tune the adjustable parameters
- Check to see if it makes sense
- Revise

$$D_{ic}(t) = \left(\frac{A(t) \times CaO(\%) + B(t) \times Na_2O_e(\%)}{SiO_2(\%)} \right)$$

Physics based model

- Pick a reasonable model with adjustable parameters
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$$D_{ic}(t) = \left(\frac{A(t) \times CaO(\%) + B(t) \times Na_2O_e(\%)}{SiO_2(\%)} \right)$$

AI models

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?



Client: Mr. Tom Hendrix
The SEFA Group
P.O. Box 6
Moncks Comer, SC 29461

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

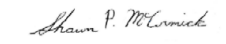
REPORT OF FLY ASH TESTS				
Sample I.D. No.: MC043020		Date Sampled: April 30, 2020		
Manufacturer: McMeekin Station (Thermally Beneficiated)		Date Received: May 6, 2020		
Chemical Analysis	Results (wt%)	Specification (Class F)		
		ASTM C618-19	AASHTO M295-19	
Silicon Dioxide (SiO ₂)	54.4	----	----	
Aluminum Oxide (Al ₂ O ₃)	27.2	----	----	
Iron Oxide (Fe ₂ O ₃)	6.82	----	----	
Sum of Silicon Dioxide, Iron Oxide & Aluminum Oxide (SiO ₂ +Al ₂ O ₃ +Fe ₂ O 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 ₂ O)	0.29	----	----	
Potassium Oxide (K ₂ O)	2.52	----	----	
"Sodium Oxide Equivalent (Na ₂ O+0.658K ₂ O)"	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 ₂ O) as Available Alkalies	0.10	----	----	
Potassium Oxide (K ₂ O) as Available Alkalies	1.04	----	----	
Available Alkalies as "Sodium Oxide Equivalent (Na ₂ O+0.658K ₂ O)"	0.78	----	1.5 % max.*	
Physical Analysis		Test Date		
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)
At 28 Days:				
Control Average, psi: 5870	Test Average, psi: 5560	6/16/20	95%	75 % min. [†] (of control)
Water Requirements (Test H ₂ O/Control H ₂ O)				
Control, mls: 242	Test, mls: 234	5/19/20	97%	105% max. [†] (of control)
Autoclave Expansion:	5/13/20	-0.04%	± 0.8 % max.	± 0.8 % max.
Uniformity Requirements		Test Date		
Specific Gravity:	2.32	Average: 2.33	5/13/20	-0.4%
% Retained #325 Sieve:	16.1	Average: 14.2	5/13/20	1.9%

[†] 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



SGS TEC SERVICES
235 Buford Drive | Lawrenceville GA 30046
770-995-8000 | www.tecservices.com



Bulk oxides

	Mass %
SiO ₂	36.2
Al ₂ O ₃	21.7
Fe ₂ O ₃	5.3
CaO	23.1
MgO	5.3
SO ₃	0.6
Na ₂ O	3.5
K ₂ O	1.0
TiO ₂	0.8
P ₂ O 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

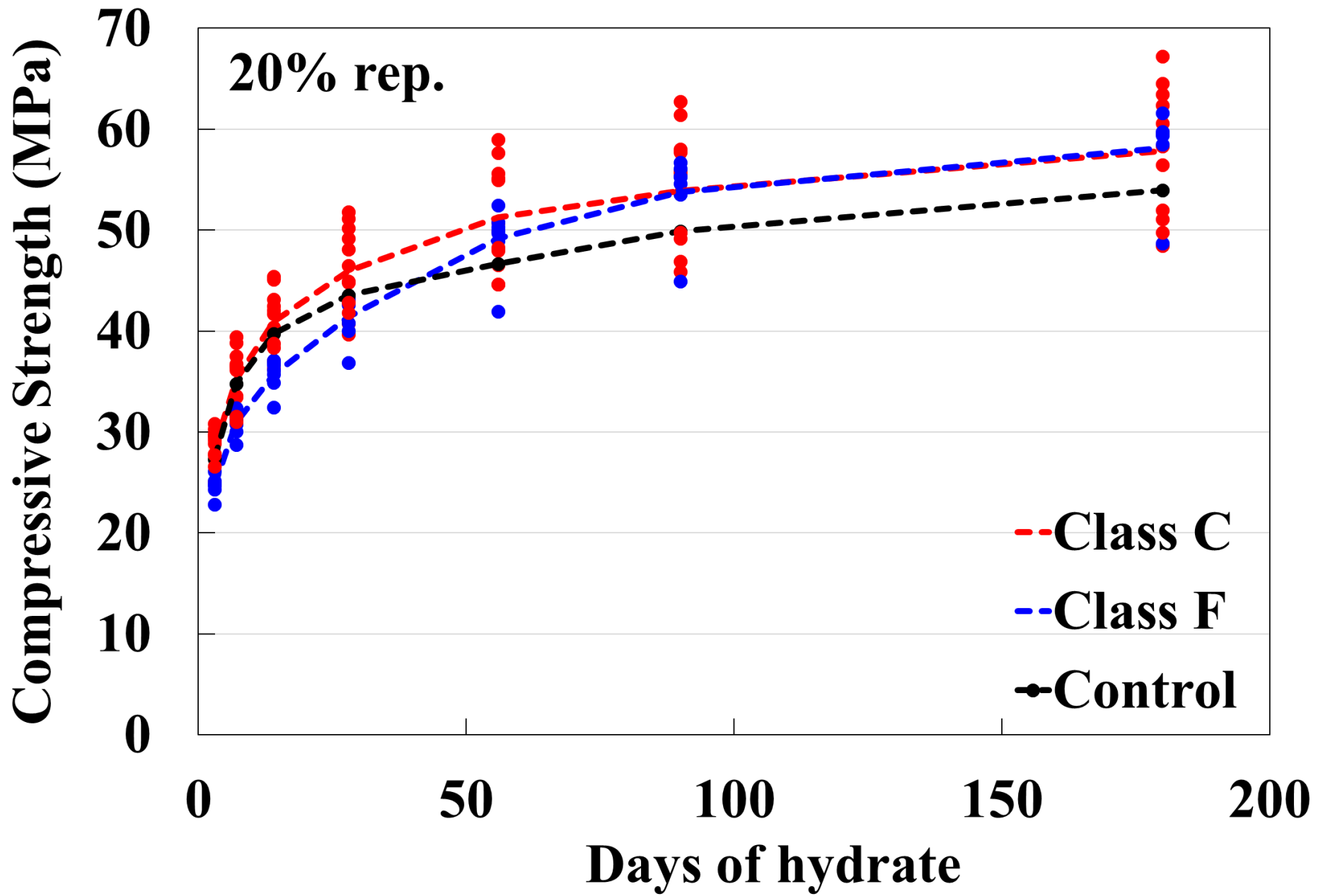
Class 3: $>$ portland cement $+ 1$ std

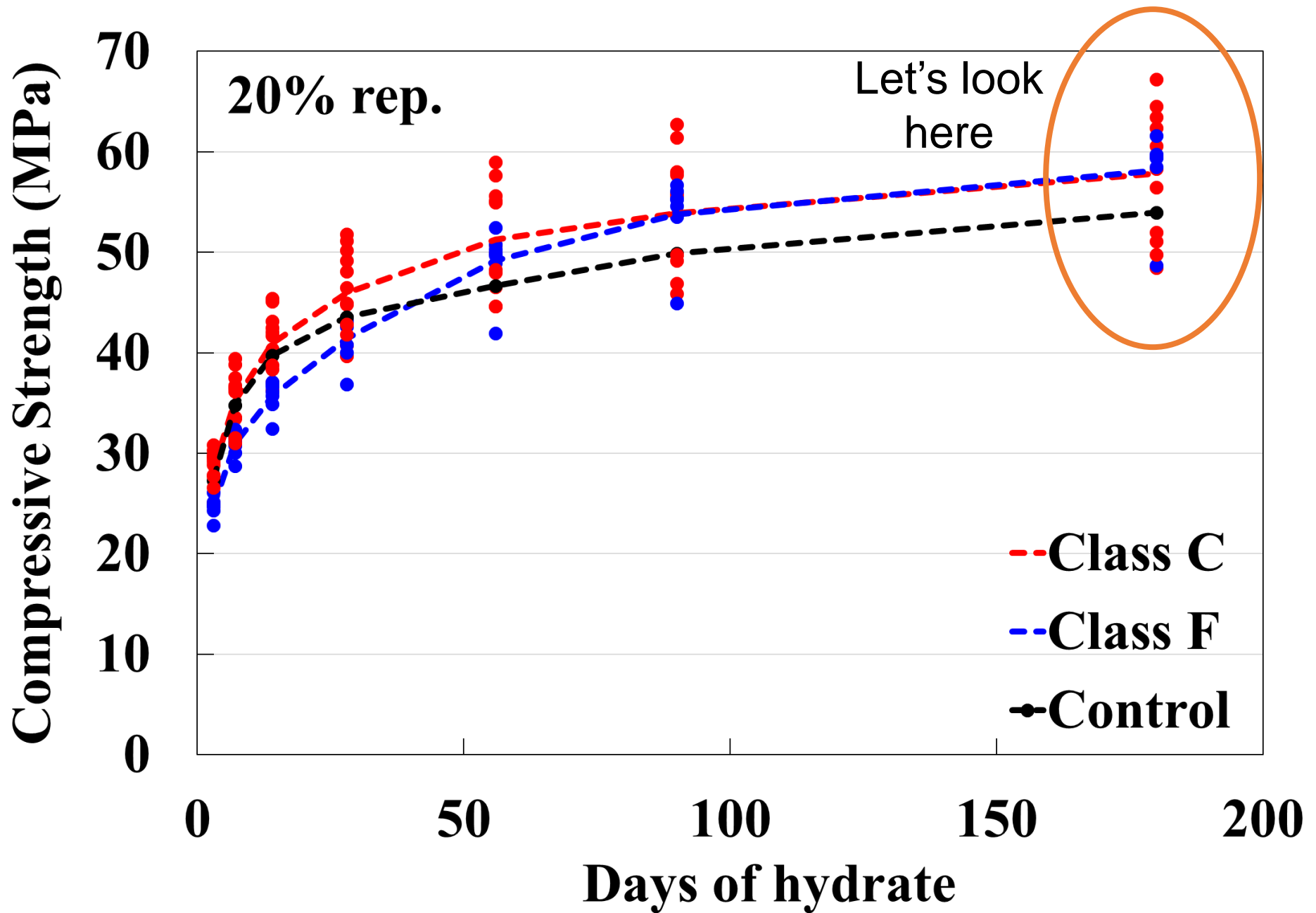
Classification Steps

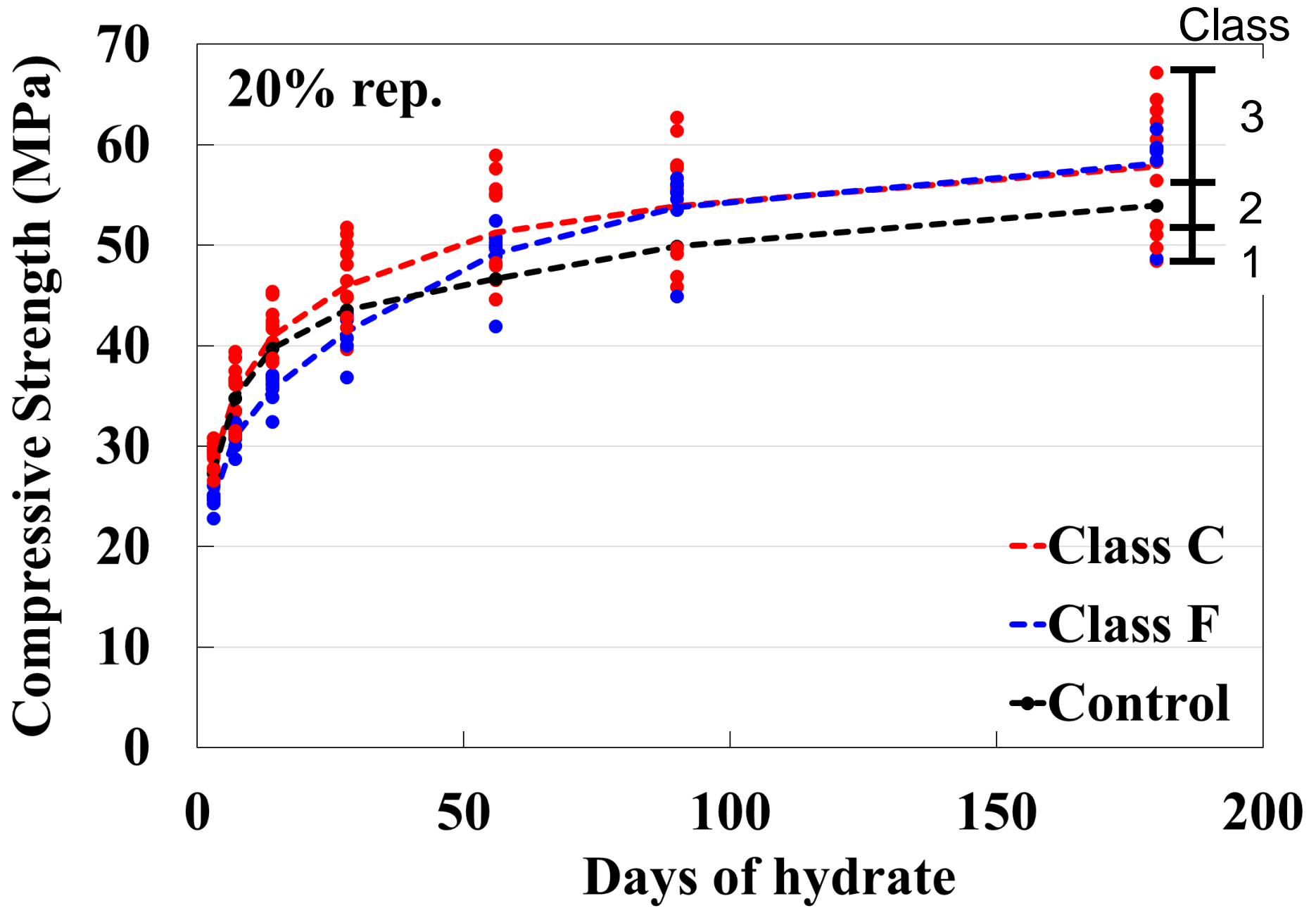
How does a concrete mixture with fly ash compare to a mixture with only portland cement?

Create performance classes

Class 1:	< OPC	- 1 std
Class 2:	Same as OPC	+/- 1 std
Class 3:	> OPC	







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)

Leave Out X Cross Validation (LOXCV)

For $x = 1$

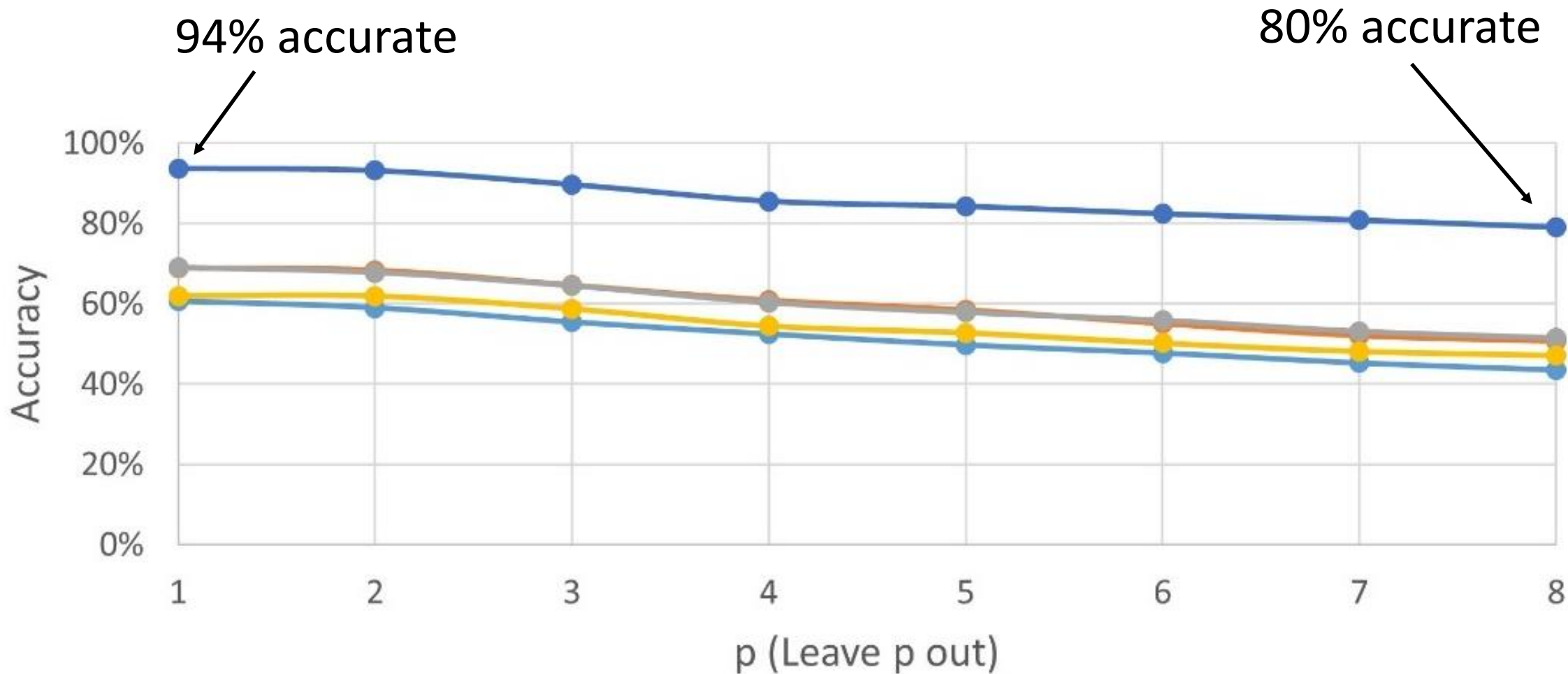
Use 43 ($44-x$ or $44-1$) observations as the training set and the remaining observation to check.

Repeat this 43 times and report the % accuracy

For $x = 2$

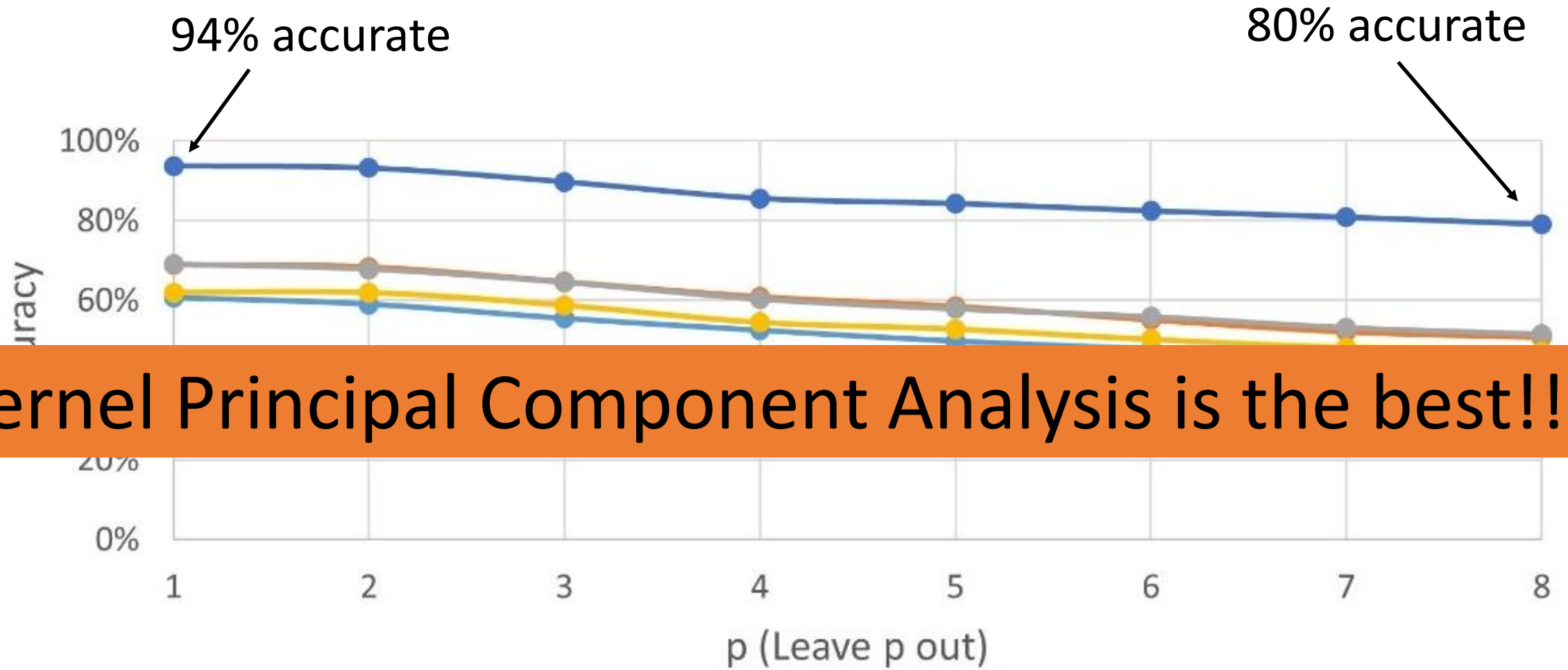
Use 42 observations as the training set and repeat this 946 times and report the % accuracy.

$${}^n C_r = \frac{n!}{(n-r)! r!}$$



Decision Trees LDA SVM KNN KPCA

Compressive strength 20% replacement all time periods.



Kernel Principal Component Analysis is the best!!!

Decision Trees LDA SVM KNN KPCA

Compressive strength 20% replacement all time periods.

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%

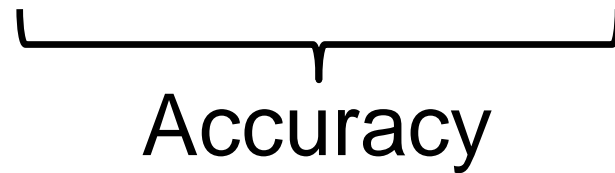
Accuracy

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 Kernel 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.

Fly Ash Performance Calculator

Chemical Components (by mass %)	
SiO ₂	36.2
Al ₂ O ₃	21.7
Fe ₂ O ₃	5.4
CaO	23.2
MgO	5.4
SO ₃	.7
Na ₂ O	3.6
K ₂ O	1
TiO ₂	.8
P ₂ O ₅	1.9
SrO	.2
Total	100.1

Calculate

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

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

Diffusion Coefficient		
Fly Ash Replacement by Mass	20%	40%
45d	Higher	Lower
90d	Higher	Lower
135d	Higher	Higher
200d	Same	Same
250d	Same	Same
500d	Same	Lower
700d	Higher	Lower

Heat of Hydration at 48 h		
Fly Ash Replacement by Mass	20%	40%
	> 165 J/g	135 J/g — 165 J/g

Fly Ash Performance Calculator

Add bulk oxide content here

Chemical Components (by mass %)	
SO ₂	36.2
Al ₂ O ₃	21.7
Fe ₂ O ₃	5.4
CaO	23.2
MgO	5.4
SO ₃	.7
Na ₂ O	3.6
K ₂ O	1
TiO ₂	.8
P ₂ O ₅	1.9
SrO	.2
Total	100.1

Calculate

Compressive Strength		
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45d	Higher	Lower
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250d	Same	Same
500d	Same	Lower
700d	Higher	Lower

Heat of Hydration at 48 h		
Fly Ash Replacement by Mass	20%	40%
	> 165 J/g	135 J/g — 165 J/g

Predicted performance here

Fly Ash Performance Calculator

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250d	Same	Same
500d	Same	Lower
700d	Higher	Lower

Heat of Hydration at 48 h		
Fly Ash Replacement by Mass	20%	40%
	165 J/g	135 J/g — 165 J/g

Predicted performance here

Fly Ash Performance Calculator



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135d	Higher	Higher
200d	Same	Same
250d	Same	Same
500d	Same	Lower
700d	Higher	Lower

Heat of Hydration at 48 h		
Fly Ash Replacement by Mass	20%	40%
	165 J/g	135 J/g — 165 J/g

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?

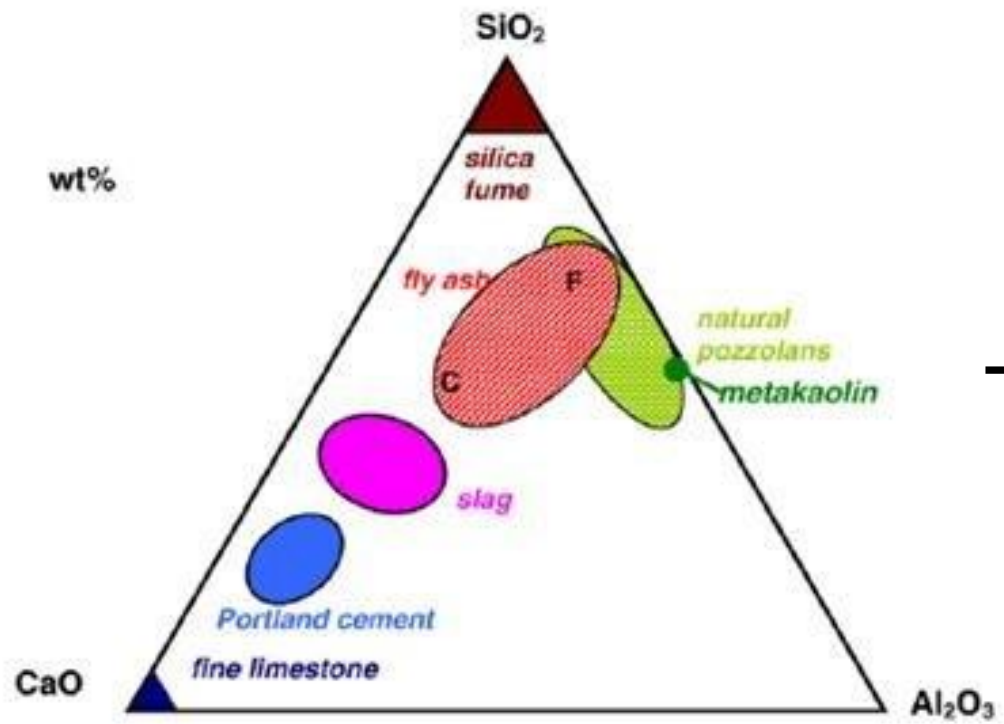
Particle size distribution is similar between these ashes

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.



Physics Based Model

Use a Physics Based Model to predict the diffusion coefficient of paste mixtures with 20% and 40% fly ash replacement.

Use a model first proposed to predict pore solution alkalinity reduction from fly ash from Shehata and Thomas.

Physics Based Model

Measure the diffusion in paste samples with the following:

0.45 w/cm

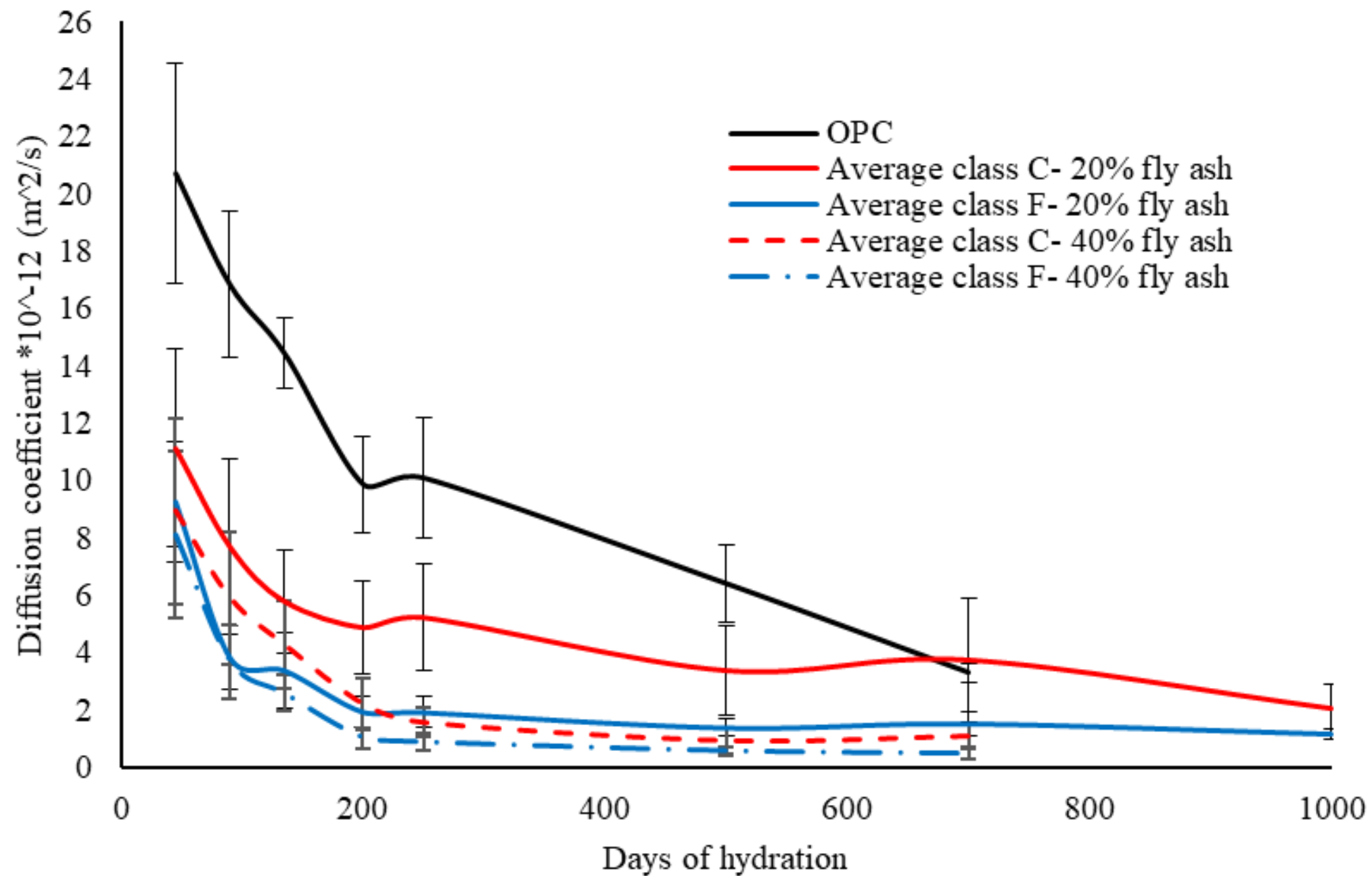
6 class F fly ashes

11 class C fly ashes

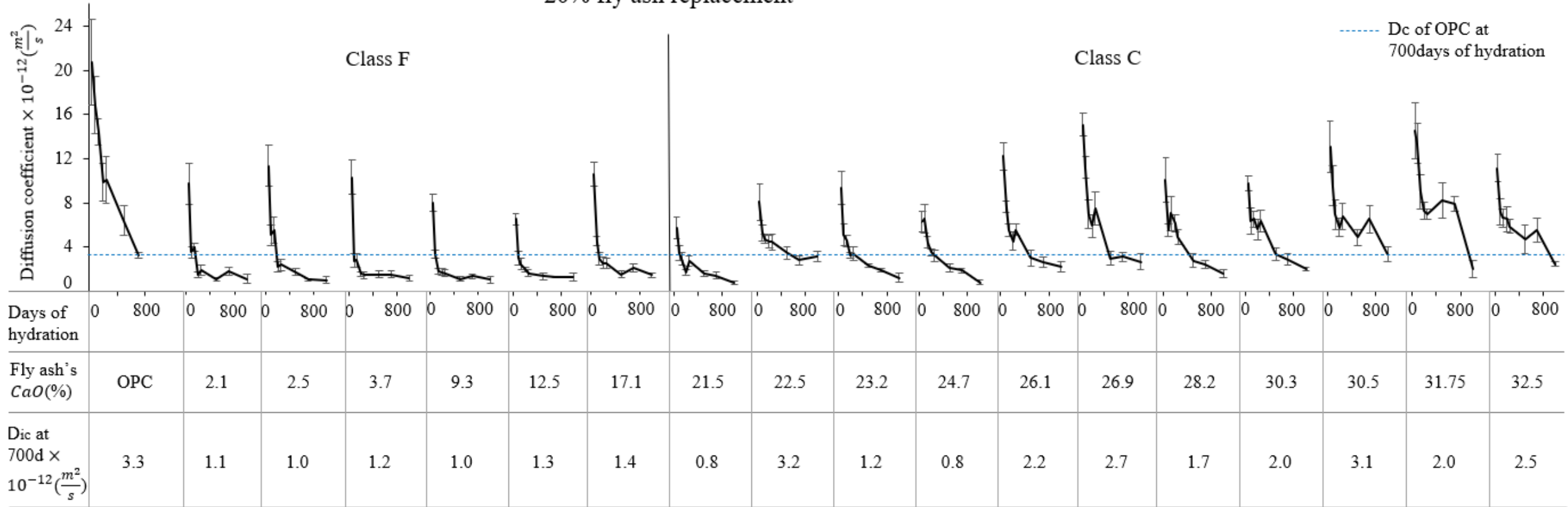
20% and 40% replacement

Samples are stored in a sealed condition.

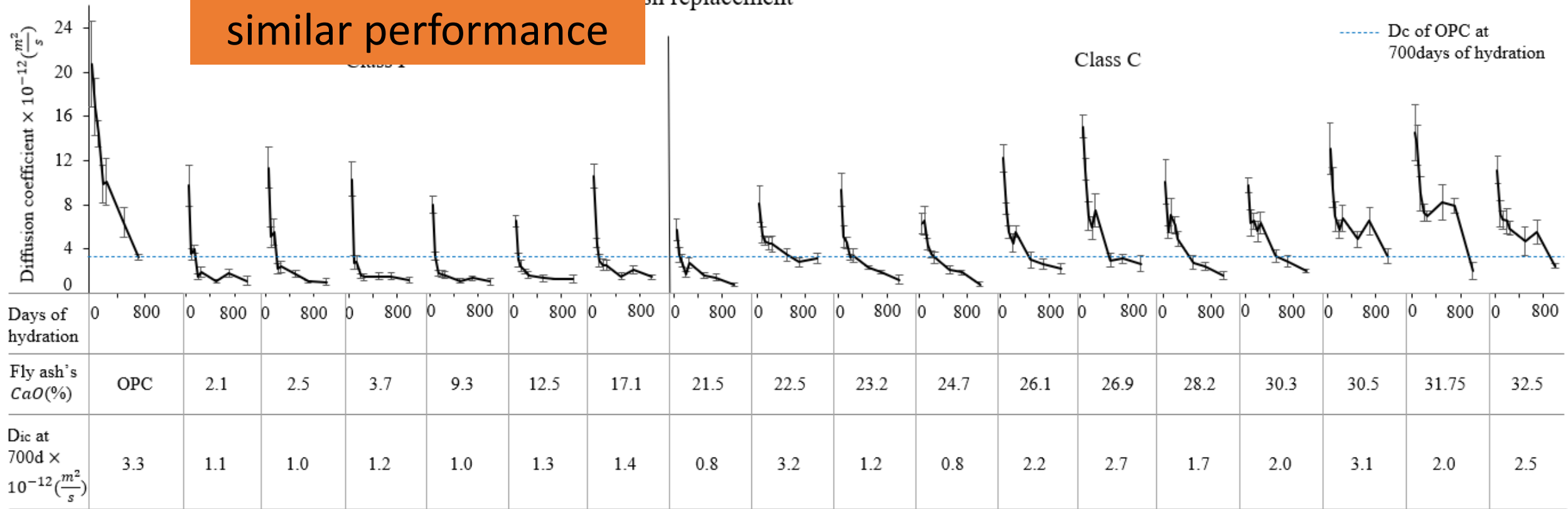
Test samples from 45 d to 3y.



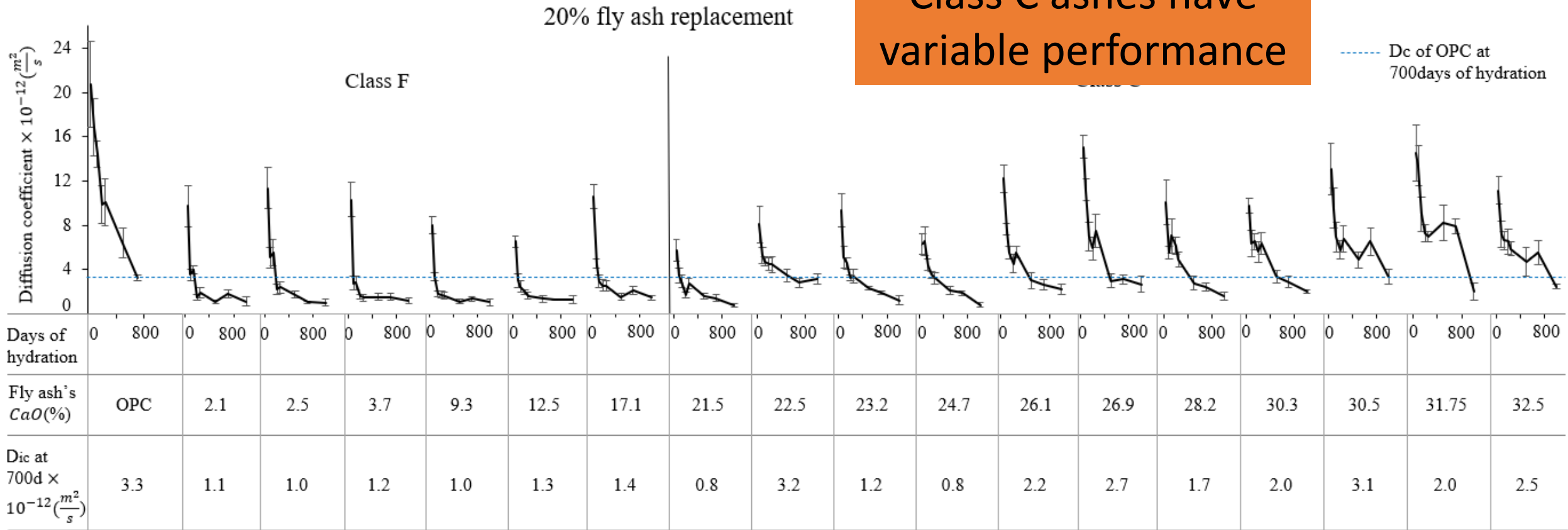
20% fly ash replacement

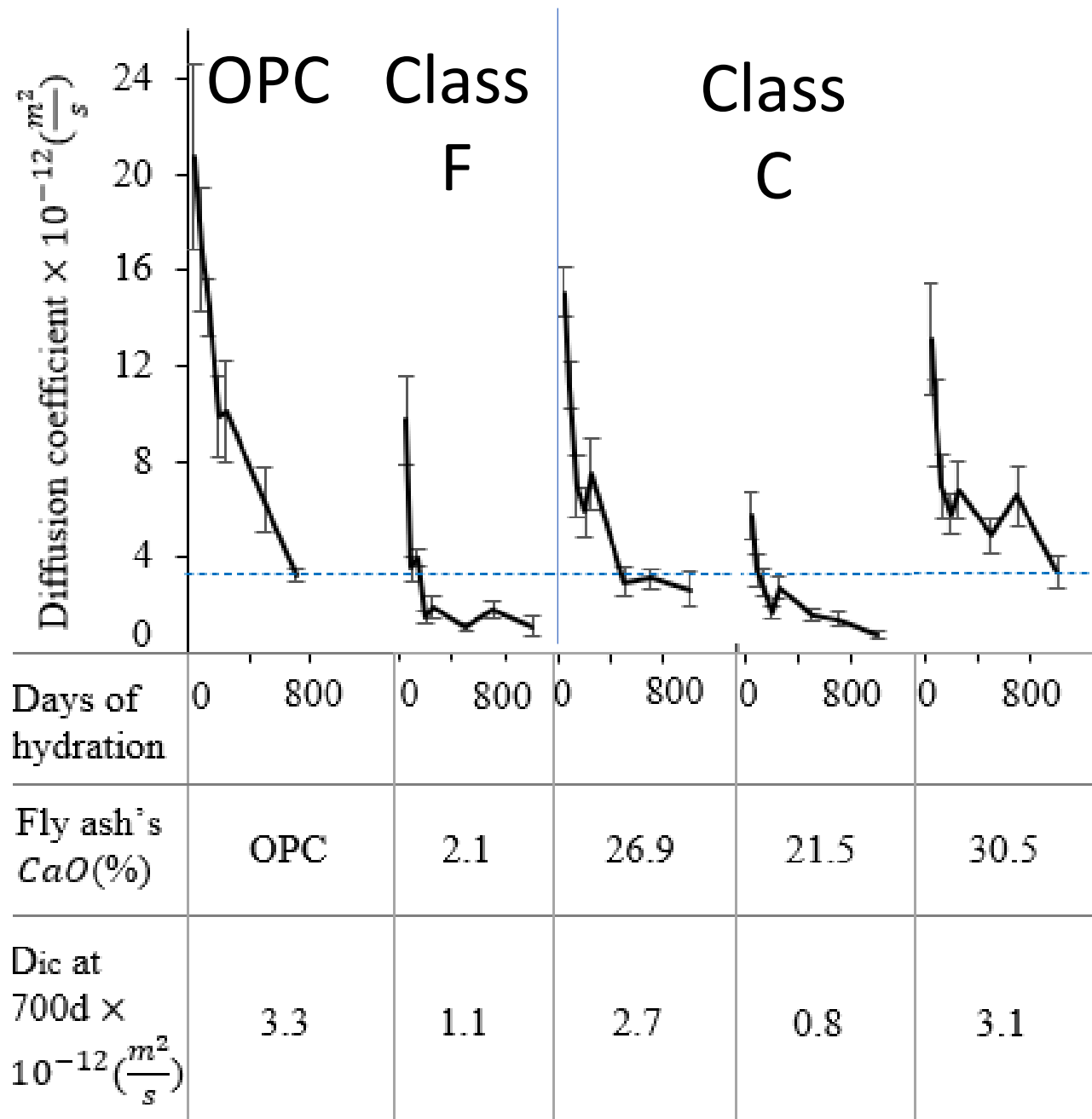


Class F ashes all have similar performance



Class C ashes have variable performance





Discussion

- All class F ashes have similar performance.
- Class C ashes have variable performance.
- Some class C are just as good as class F and many are not
- Some class C are better than OPC and some are not!

Discussion

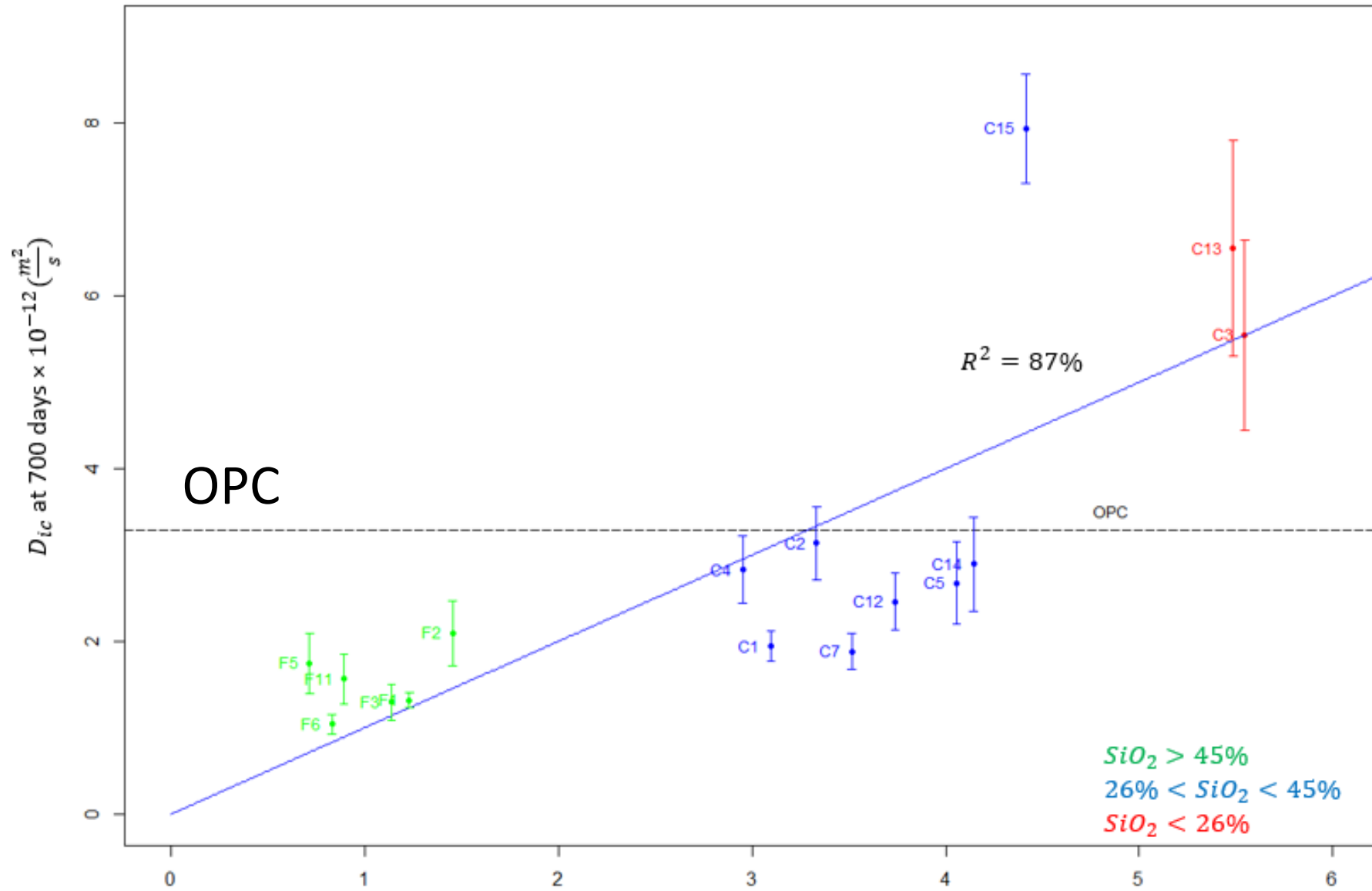
- All class F ashes have similar performance.

**It would be great if we had a model that
could predict this!**

- Some class C are just as good as class F and many are not
- Some class C are better than OPC and some are not!

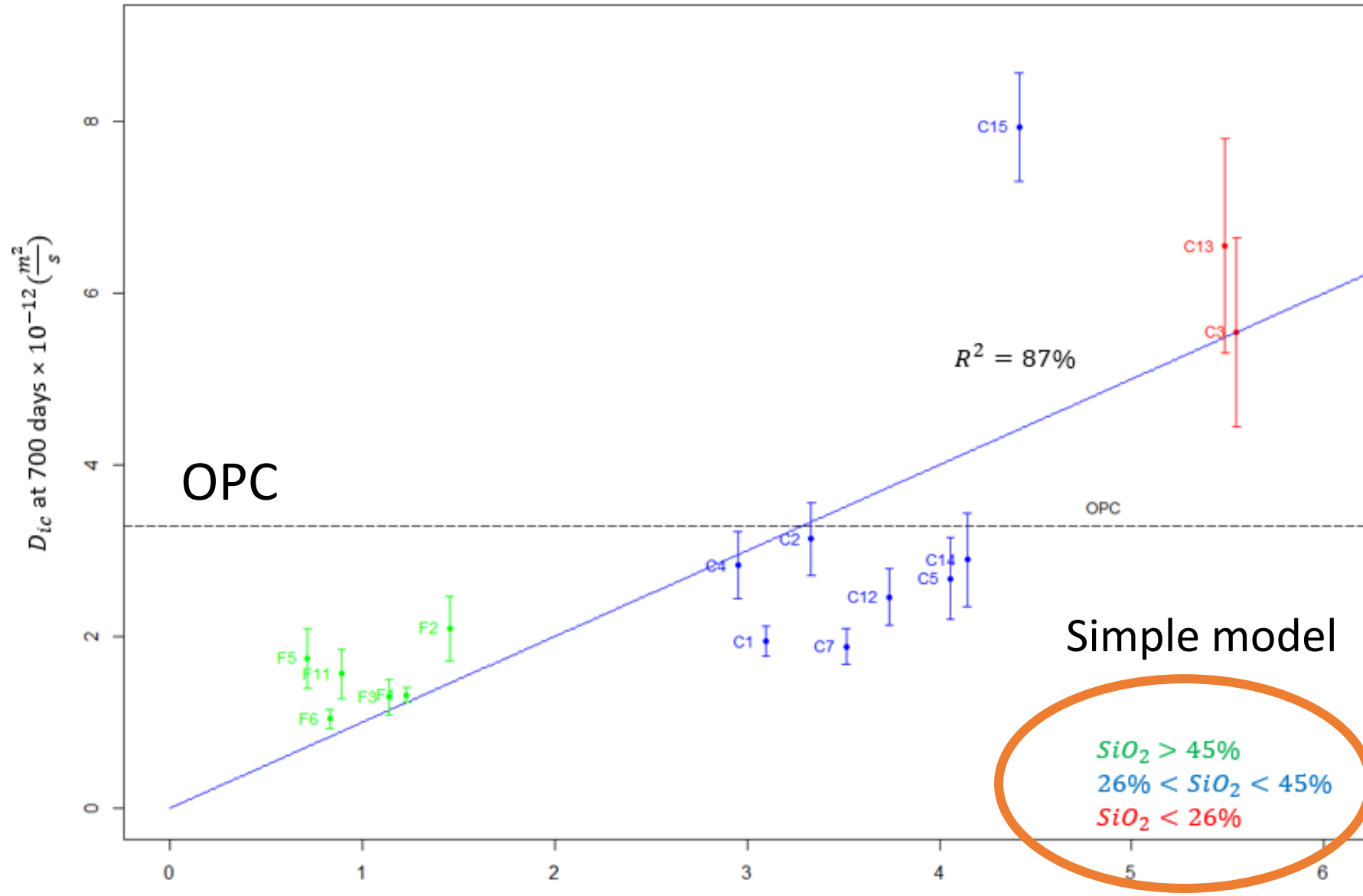
$$D_{ic}(t) = \left(\frac{A(t) \times CaO(\%) + B(t) \times Na_2O_e(\%)}{SiO_2(\%)} \right)$$

20% fly ash replacement, 700days of curing



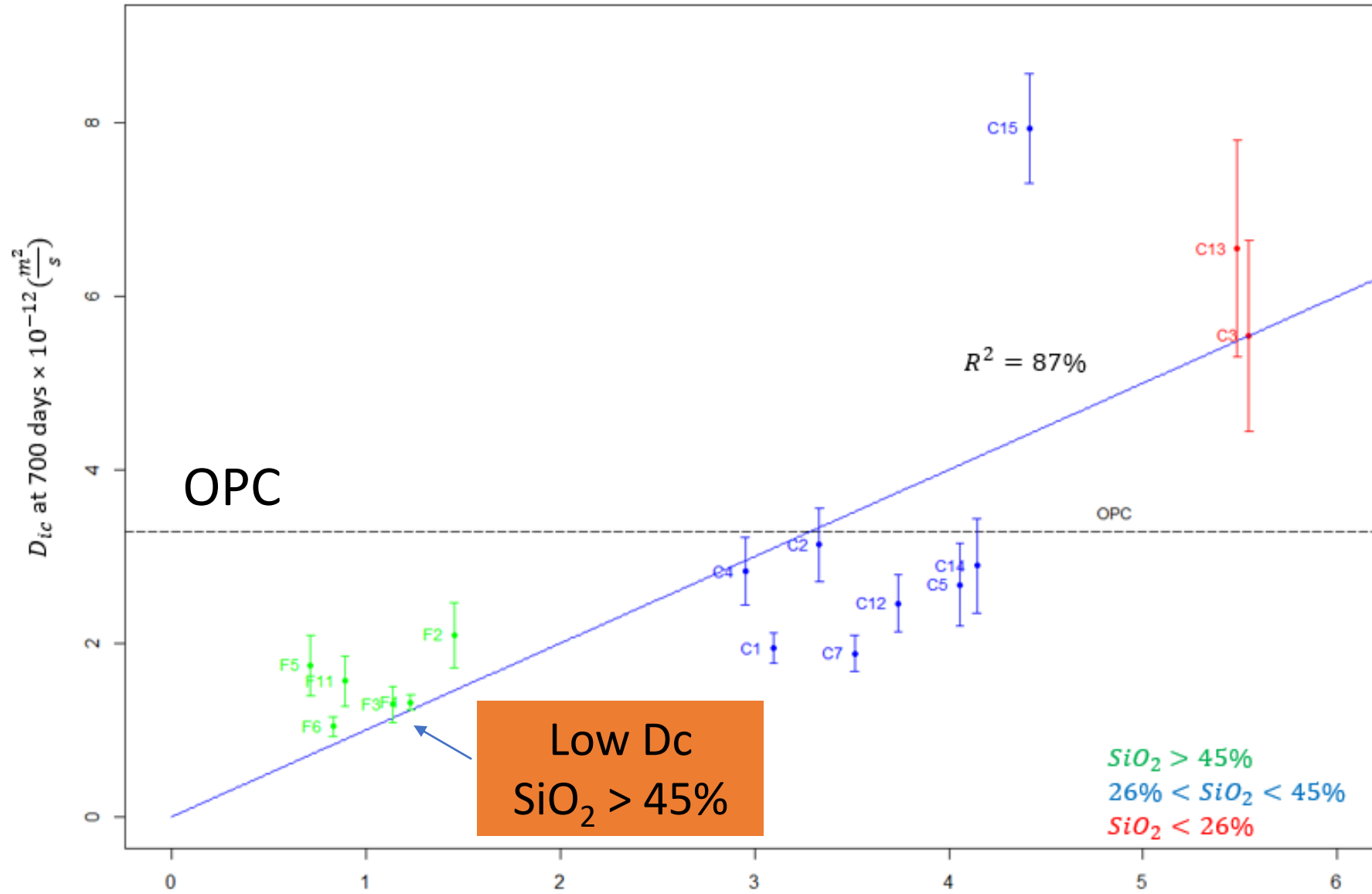
$$D_{ic}(t) = \left(\frac{3.378 \times CaO(\%) + 7.985 \times Na_2O_e(\%)}{SiO_2(\%)} \right)$$

20% fly ash replacement, 700days of curing



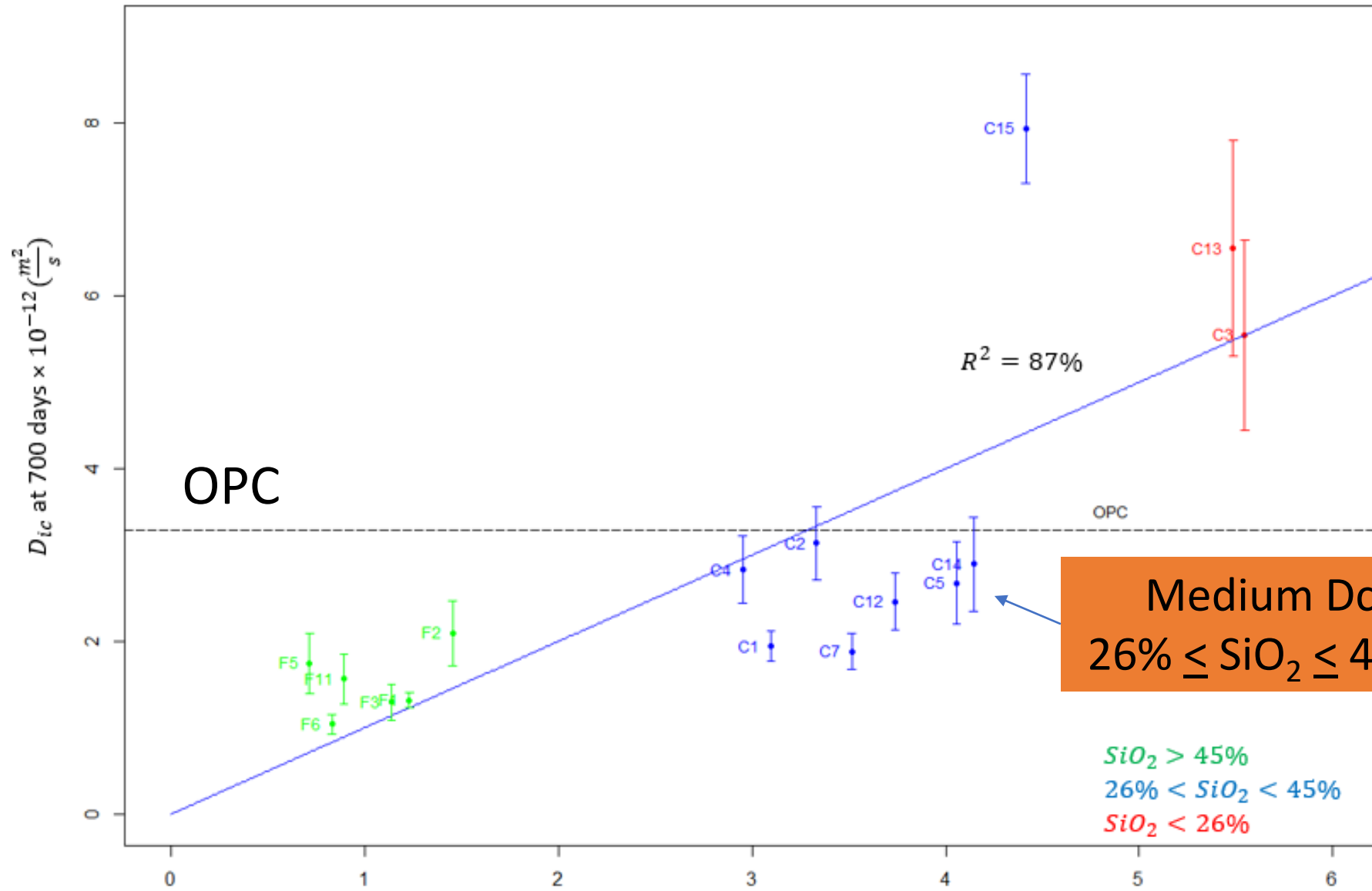
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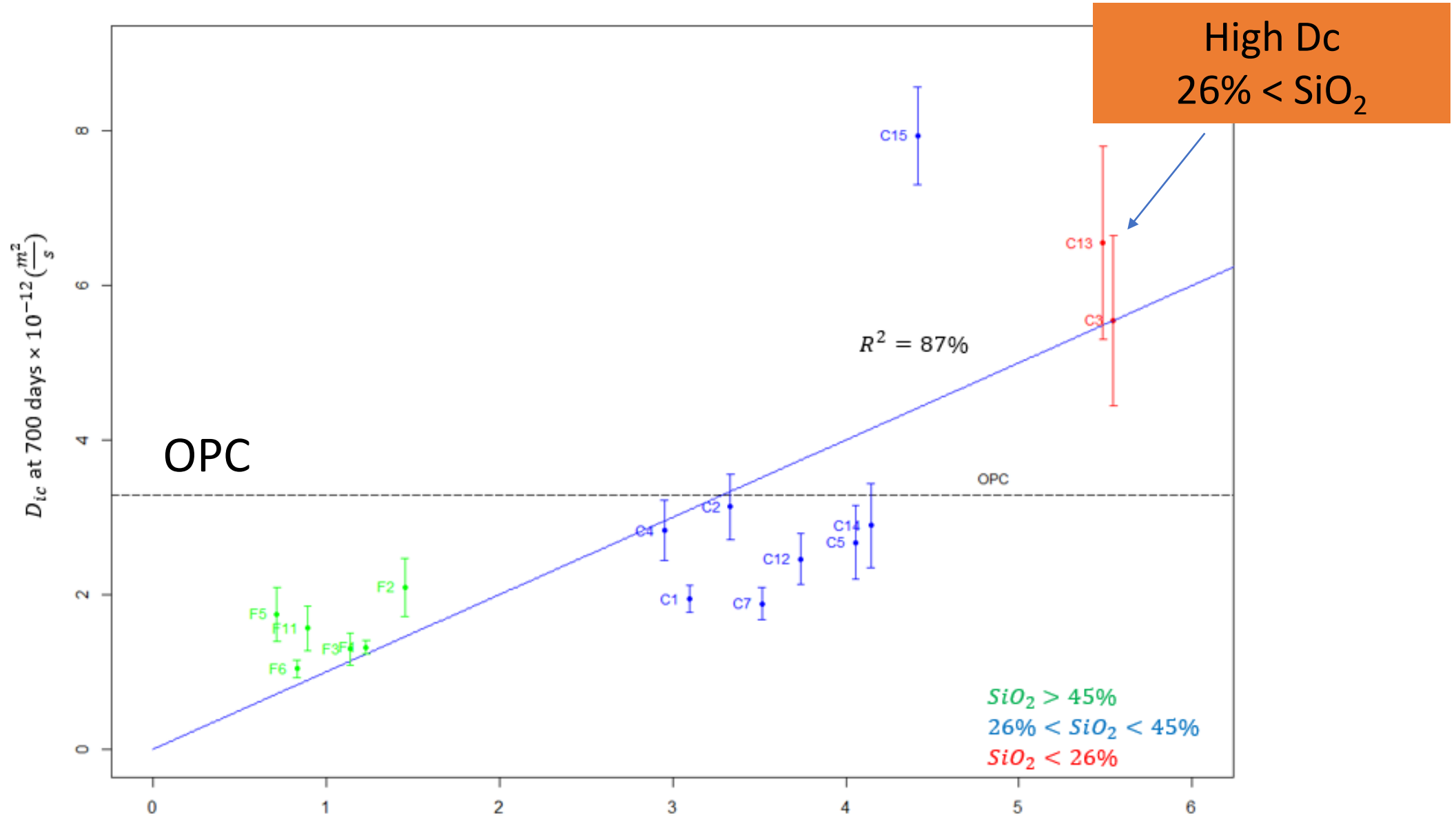


Medium Dc
 $26\% \leq SiO_2 \leq 45\%$

$SiO_2 > 45\%$
 $26\% < SiO_2 < 45\%$
 $SiO_2 < 26\%$

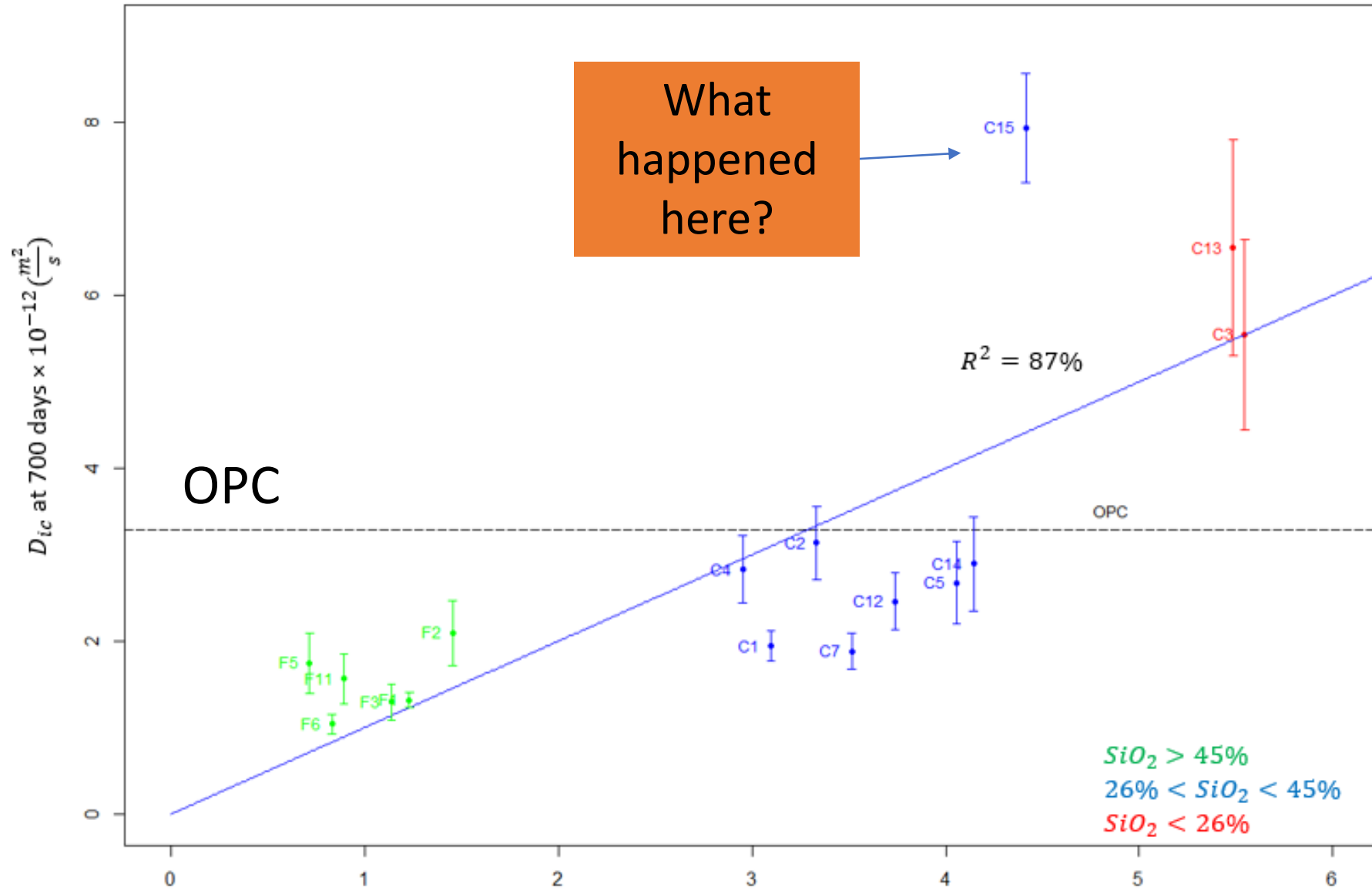
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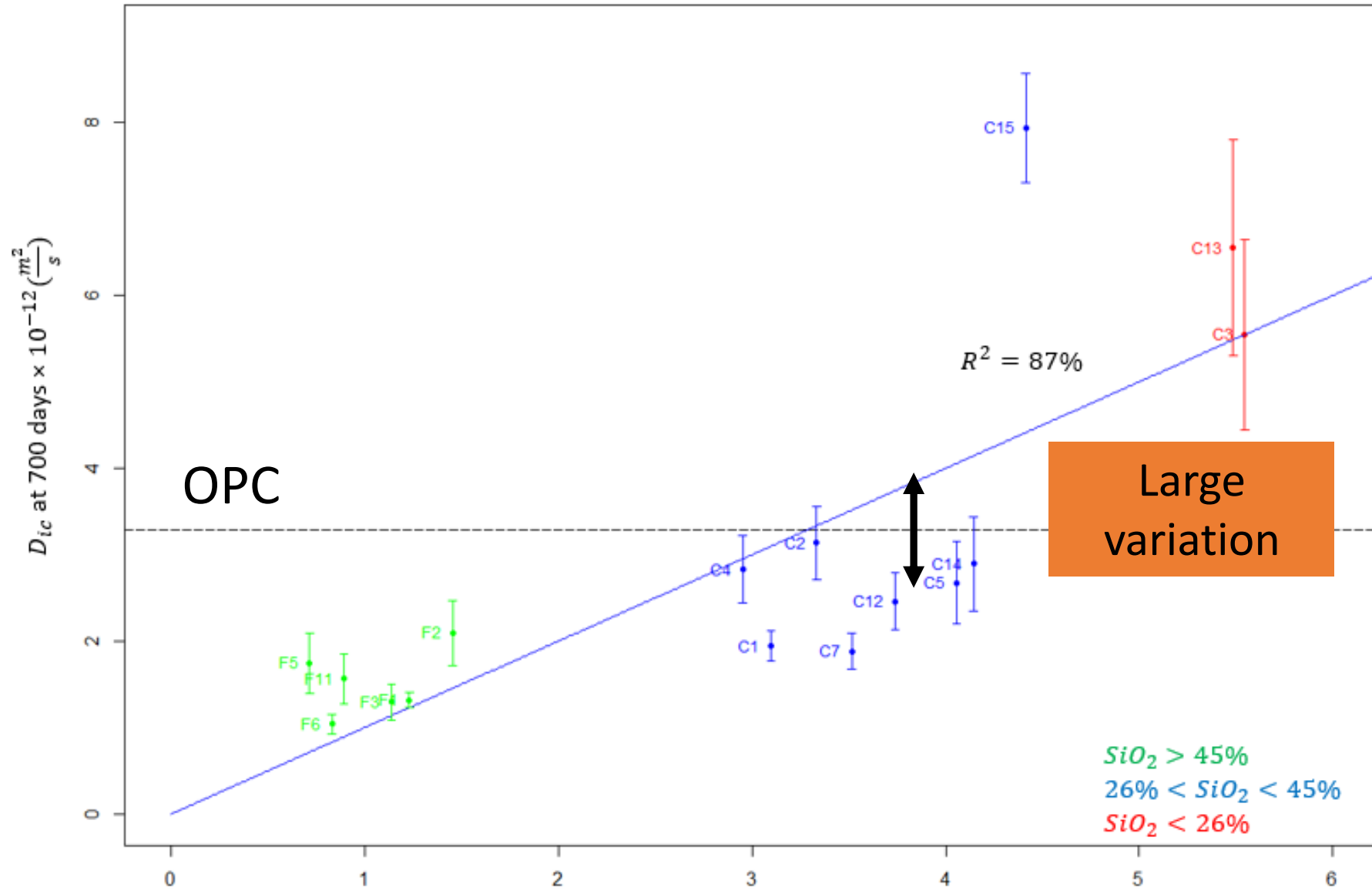
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20% fly ash replacement, 700days of curing



$$Dic(t) = \left(\frac{3.378 \times CaO(\%) + 7.985 \times Na_2O_e(\%)}{SiO_2(\%)} \right)$$

Discussion

- A Physics Based model was derived to predict the diffusion coefficient with an R^2 value of 0.87.
- A simple model based on only the SiO₂ was able to predict low, medium and high performers.
- There is one outlier and there is some variation between the predicted and measured values.

How could this be used?

You can use the amount of SiO_2 to rapidly predict high, low, and medium performance of fly ash.

If you add the CaO and the alkalies then you can get better quantitative predictions.

An Observation

- AI/ML is great but it needs a lot of data and it needs to be pointed in the right direction.
- Physics Based models are powerful but they are “restricted” to the model that use.

An Observation

- When you blend Physics and AI/ML models then they can compensate for each other
- As you restrain AI/ML models you need less data.
- There are lots of things that we “think” we understand that AI/ML will teach us that we are wrong.

An Important Statement

You are only as good as your data.

You must validate your models and be careful not to overstate their usefulness.

It is about constant improvement!!!

Conclusion

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

The Kernal PCA model can predict the performance level of both traditional and harvested fly ash for compressive strength, resistivity, diffusion, and heat of hydration.

Conclusion

The Physics Based model was also useful and provided accurate predictions with even less computation.

You should use whatever models are best for you with the data you have and based on what you want to learn.

> 98K subscribers
> 9.8M views



Structural Cracking in Reinforced Concrete

www.youtube.com/tylerley

TYLER LEY, PE, PhD

Fly Ash Performance Calculator

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Heat of Hydration at 48 h		
Fly Ash Replacement by Mass	20%	40%
	> 165 J/g	135 J/g — 165 J/g

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

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.



Purdy

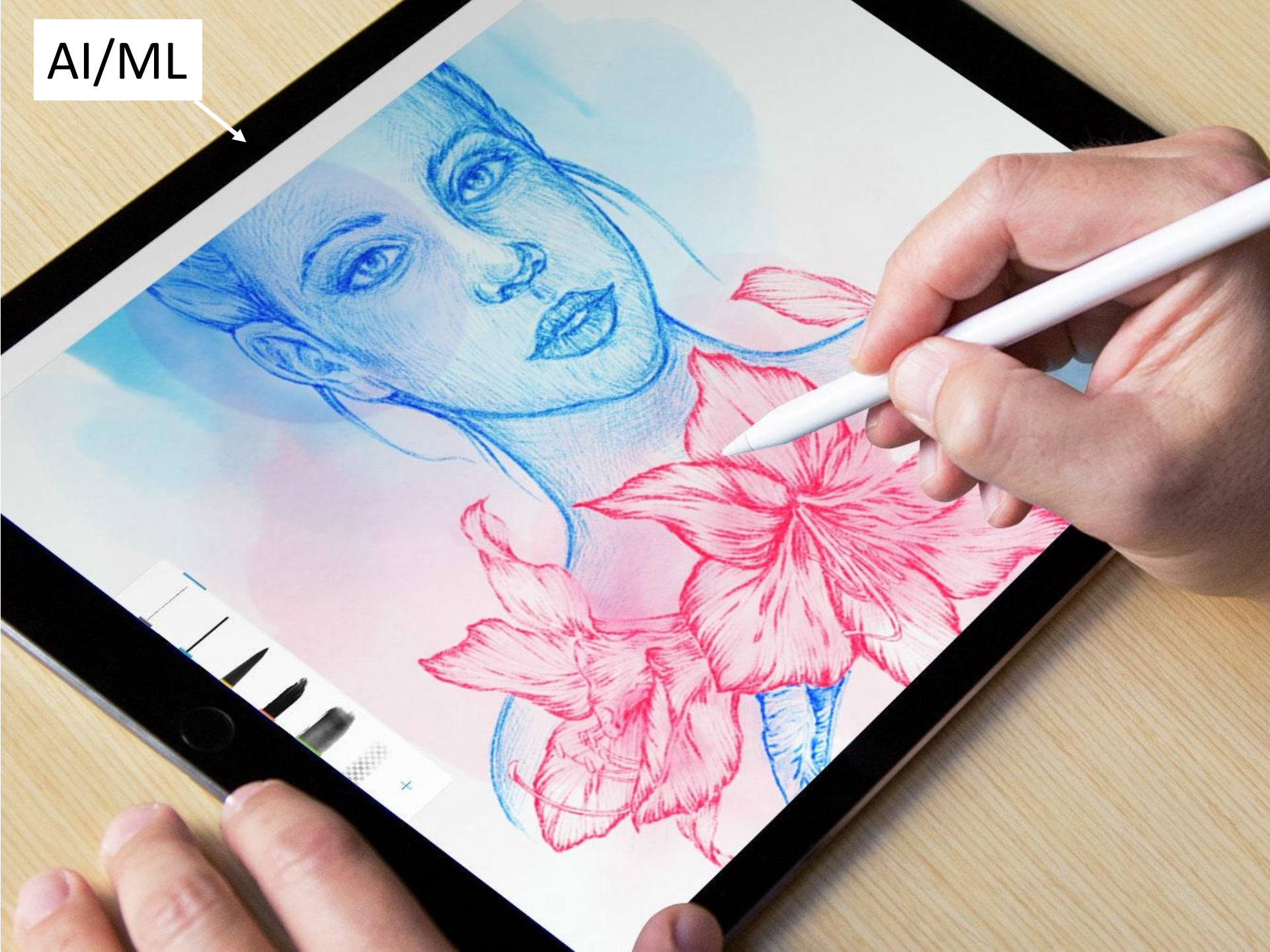
Purdy®

AI/ML





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



...



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



Tyler × DALL·E
Human & AI