
# Heat of hydration model to predict concrete temperature rise:

## Gaussian process regression links paste characteristics to mass concrete performance

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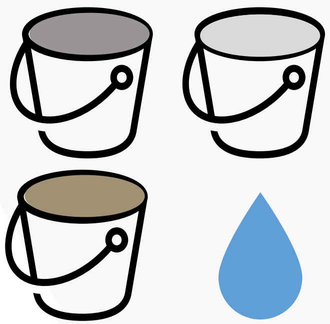
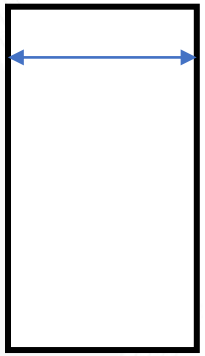
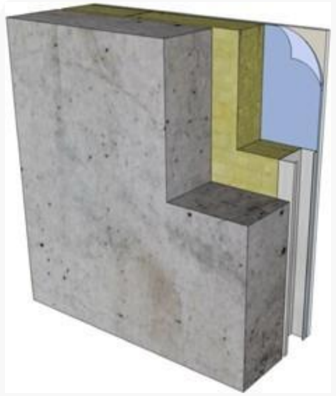
# Outline

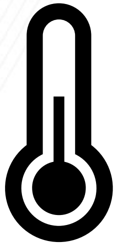
1. Mass concrete definition
2. Thermal modeling background
3. Role of machine learning
4. Mass concrete application

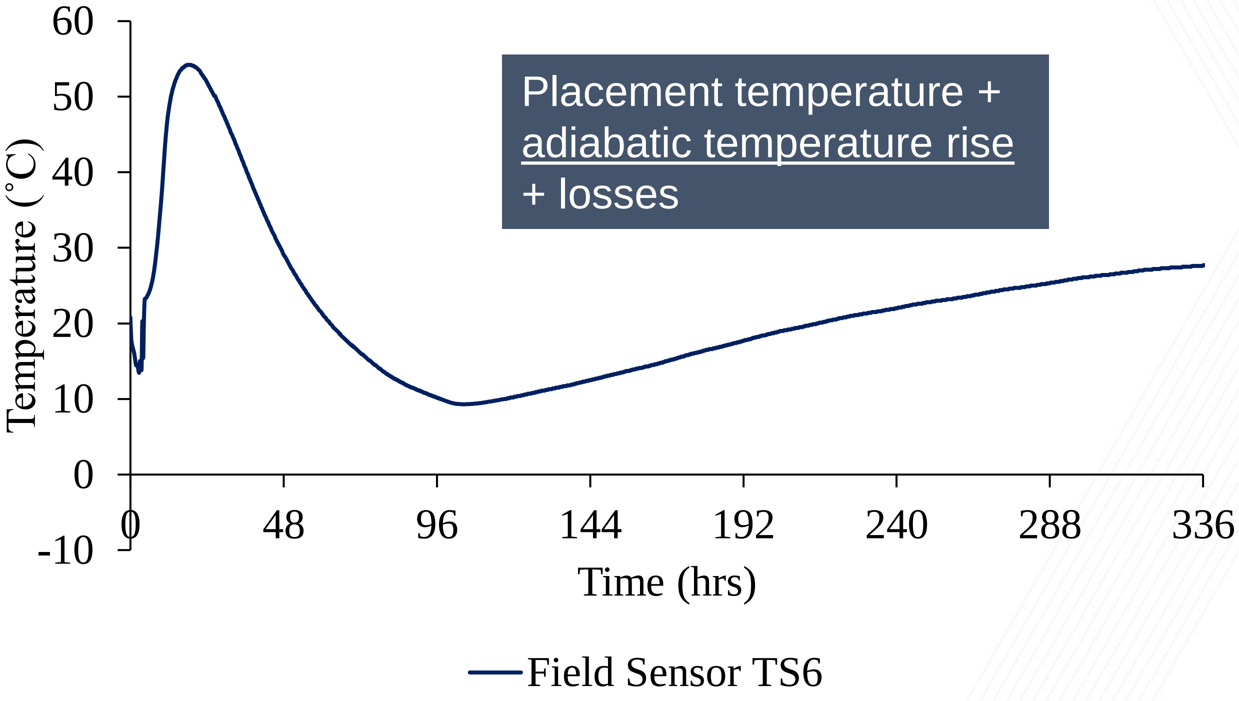
# What is mass concrete?









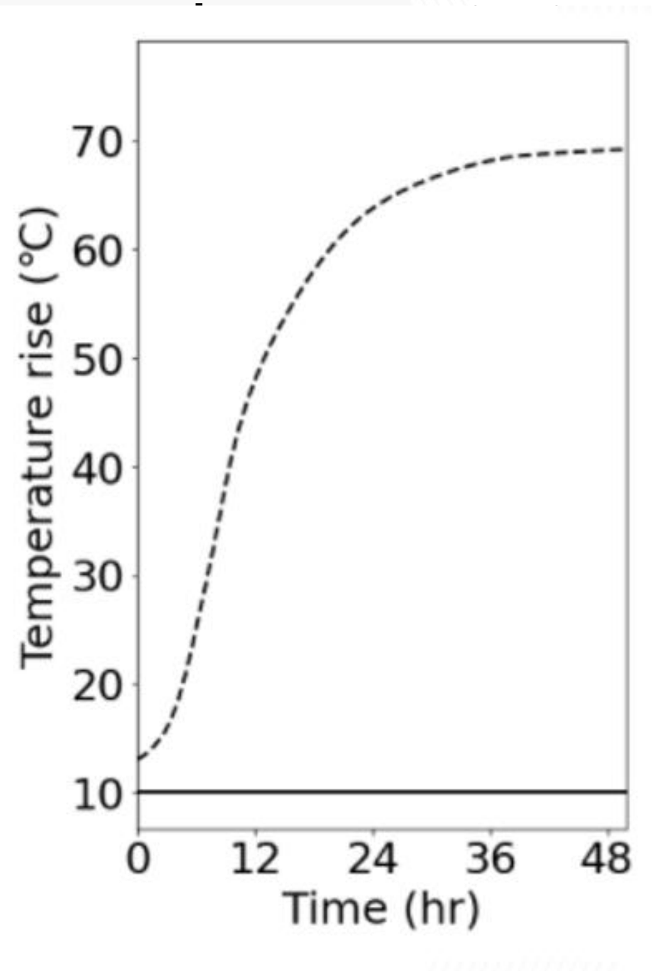


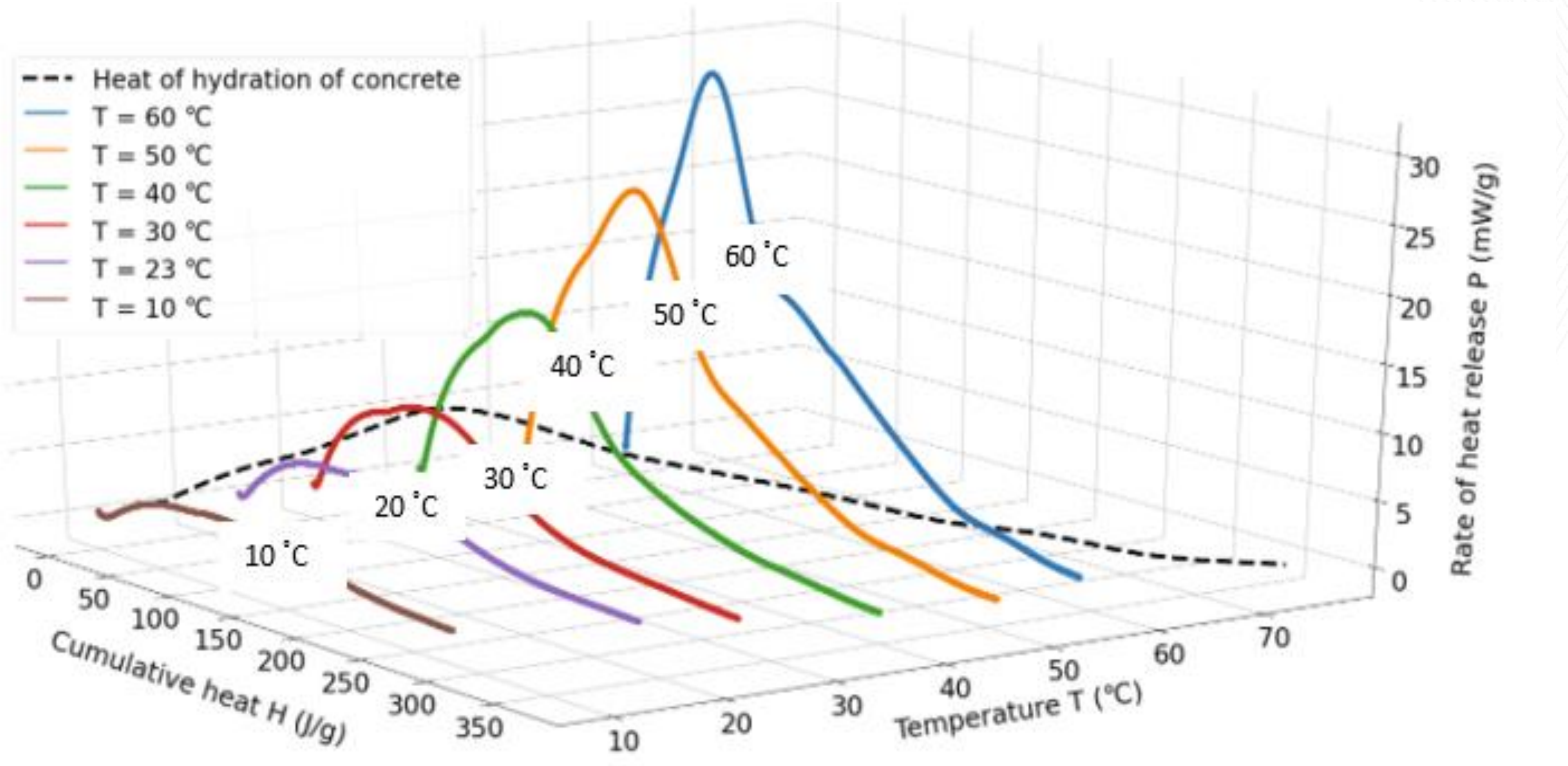

https://guides.co/g/vapor-diffusion-guide/132772

# Determination of heat of hydration

1. H and T of <u>CONCRETE</u> can be easily predicted from paste

ure



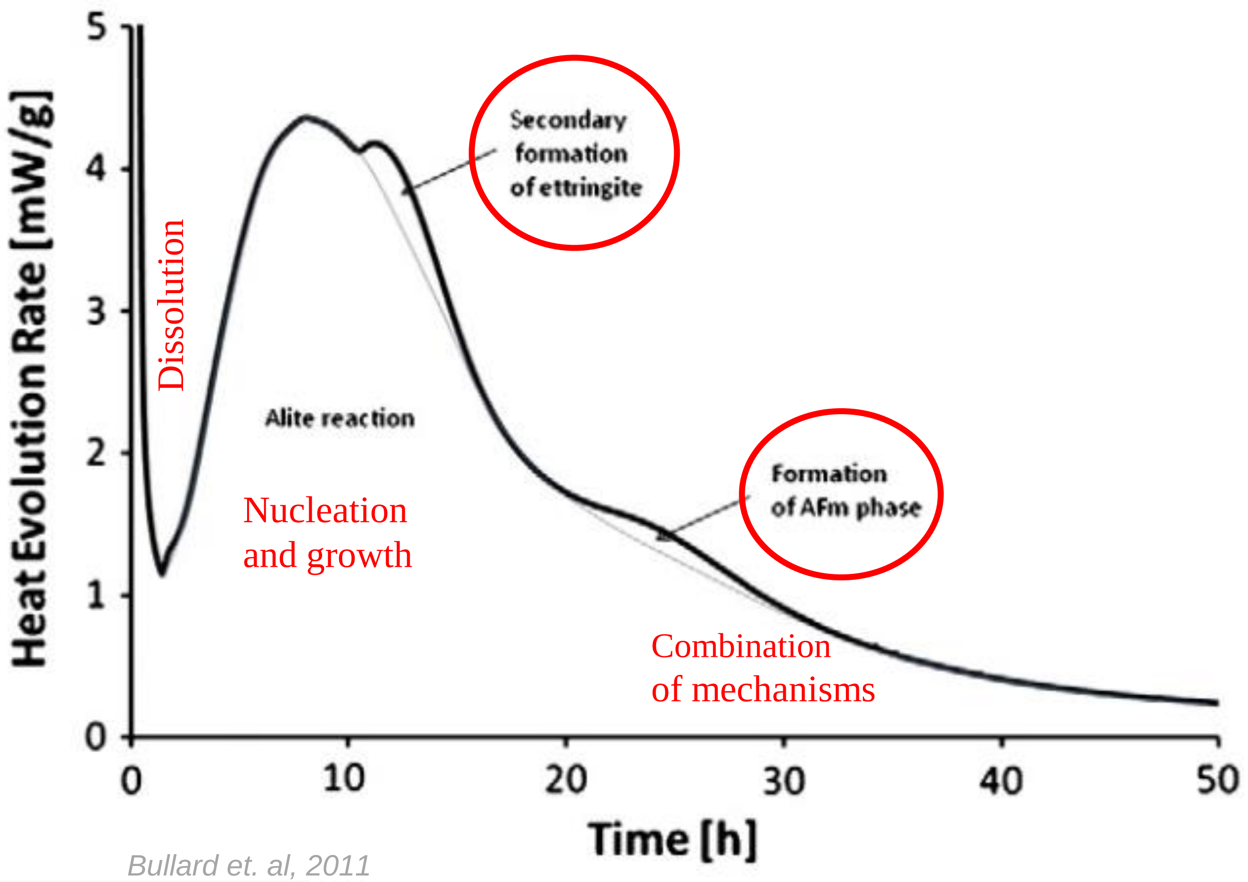




*Xu et al. (2015)*

# Objective...

How can we find the heat of hydration at different temperatures without performing isothermal calorimetry?

# Kinetic models for heat of hydration




*Bullard et. al, 2011*

- $C_3A$ + gypsum hydration
- SCMs
- Admixtures
- Models are not generalizable

# Machine learning

- 407 cumulative heat of hydration histories

| Feature | Cumulative heat |
|---|---|
| Time ↑ | ↑ |
| Temperature ↑ | ↑ |
| Fineness ↑ | ↑ |
| $C_3S$, $C_3A$ ↑ | ↑ |
| $SO_3$ ↑ | ↑ |
| MgO ↑ | ↑ |
| Alkalis ↑ | ↑ |
| w/s ↑ | ↑ |
| Fly ash ↑, FA CaO ↑ | ↓ ↑ |
| Slag ↑ | ↓ |
| Limestone ↑ | ↕ |
| Activation energy-based rate factor | Captures temperature sensitivity |



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# Gaussian process regression

Output

Input

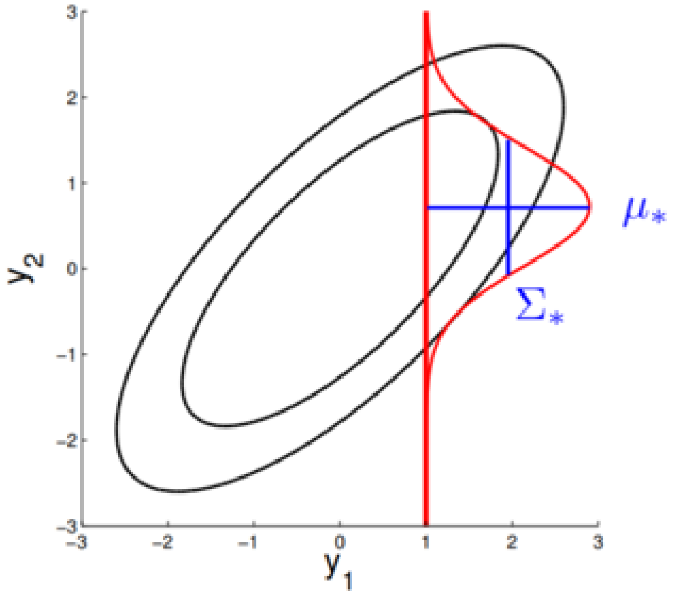
$$y = f(x)$$

In linear regression

$$y = ax + b$$

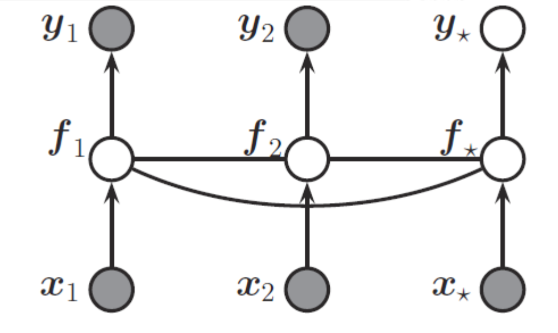
In GPR: distribution over functions at a finite set of points

- A GP assumes distribution is jointly gaussian
  - Mean $\mu(x)$
  - Covariance $\sum(x)$ which is a kernel $k$ function



# Gaussian process regression

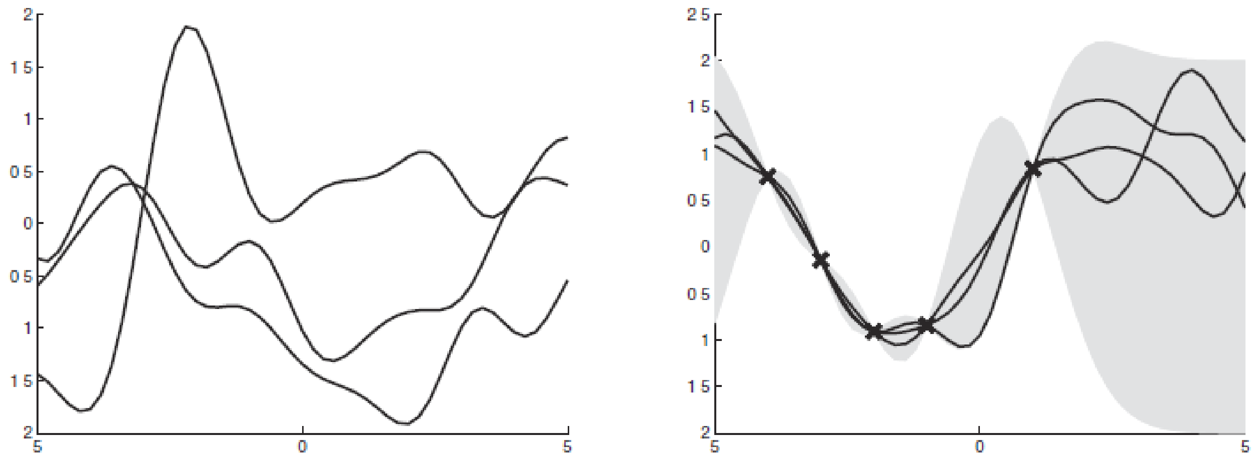
Kernels measure similarity




*Murphy, Kevin P. Machine Learning: A Probabilistic Perspective*

Prior

Posterior



(a) (b)

*Murphy, Kevin P.. Machine Learning : A Probabilistic Perspective*

Matern 3/2 kernel

$$k(x_i, x_j|\theta) = \sigma_f^2 \left(1 + \frac{\sqrt{3}\,r}{\sigma_l}\right) \exp\left(-\frac{\sqrt{3}\,r}{\sigma_l}\right)$$



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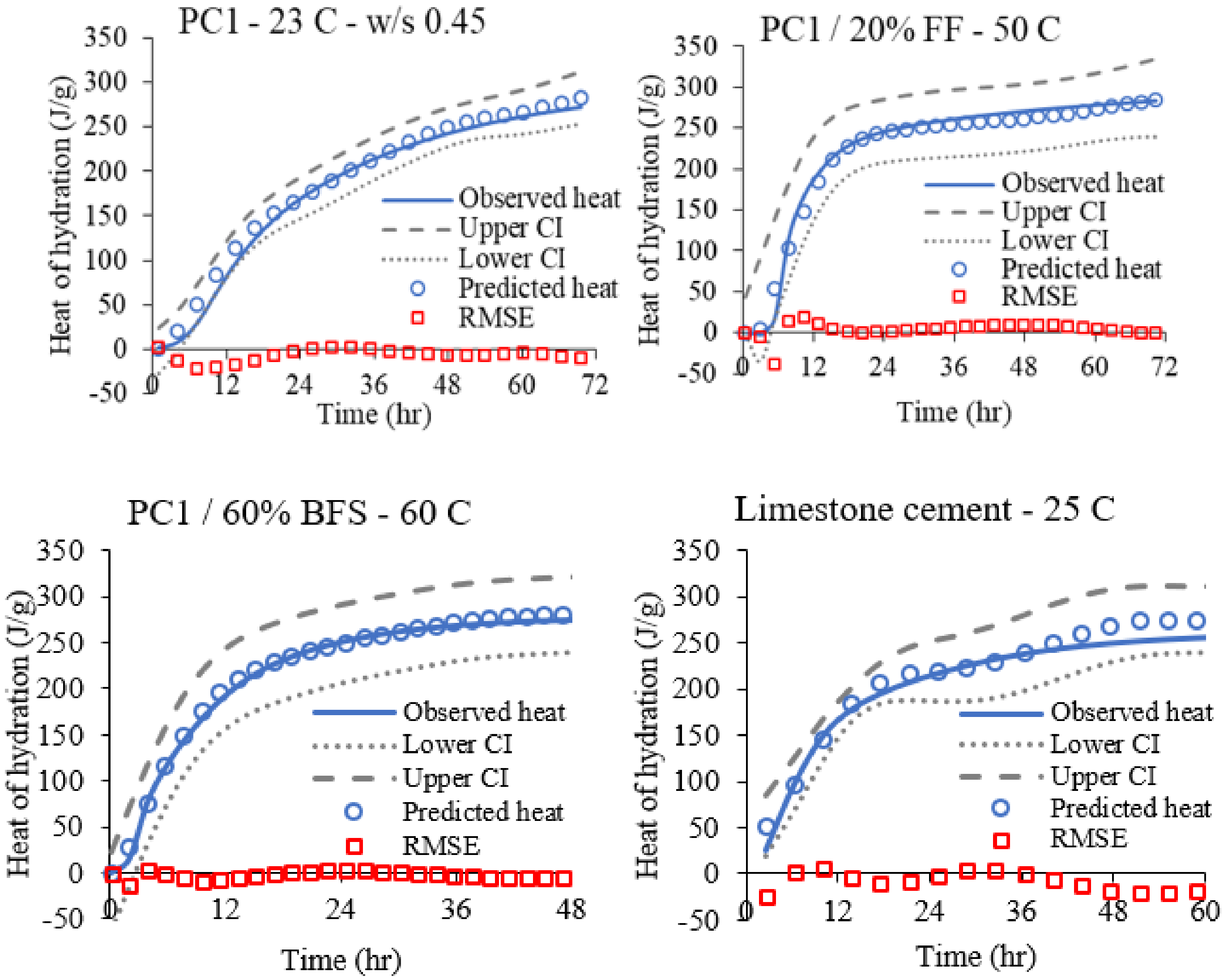
# Results

- PC: Portland cement
- FF: Class F fly ash
- BFS: Blast furnace slag



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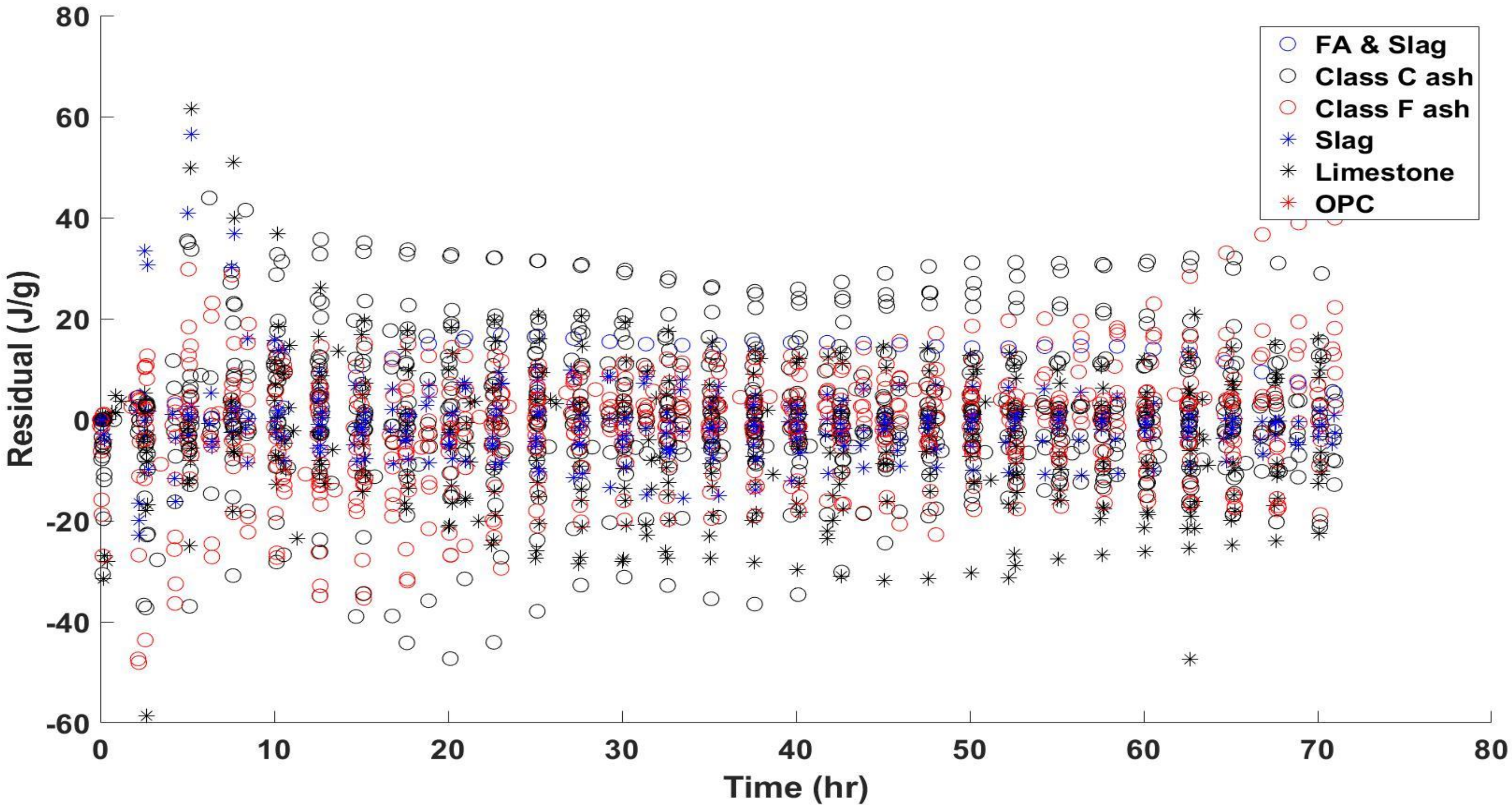
# Results

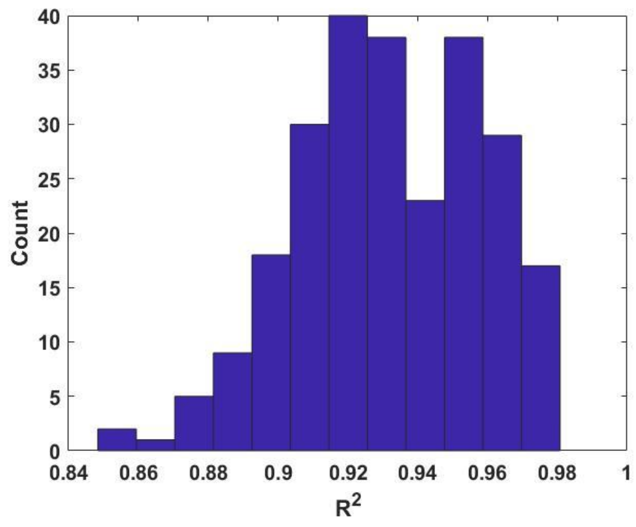


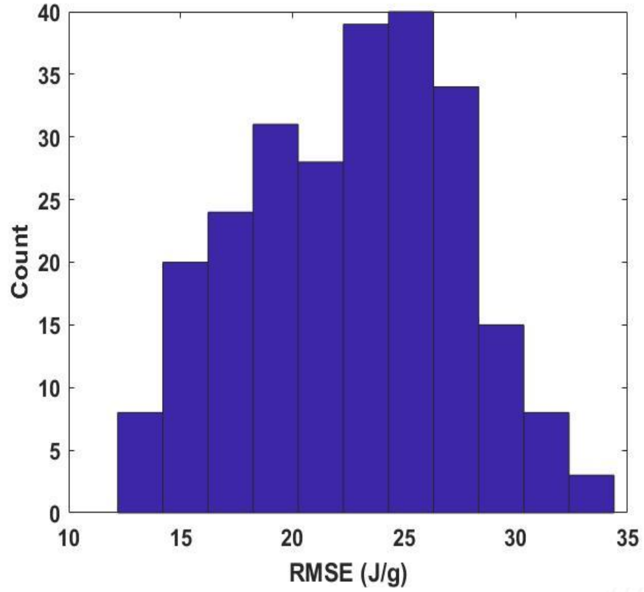
FA & Slag
Class C ash
Class F ash
Slag
Limestone
OPC
Residual (J/g)
Time (hr)
80
60
40
20
0
-20
-40
-60
0
10
20
30
40
50
60
70
80

# Model stability

- 200 iterations

| Criteria | $R^2$ | RMSE (J/g) | MAE (J/g) |
| --- | --- | --- | --- |
| **Mean** | 0.932 | 22.64 | 12.25 |



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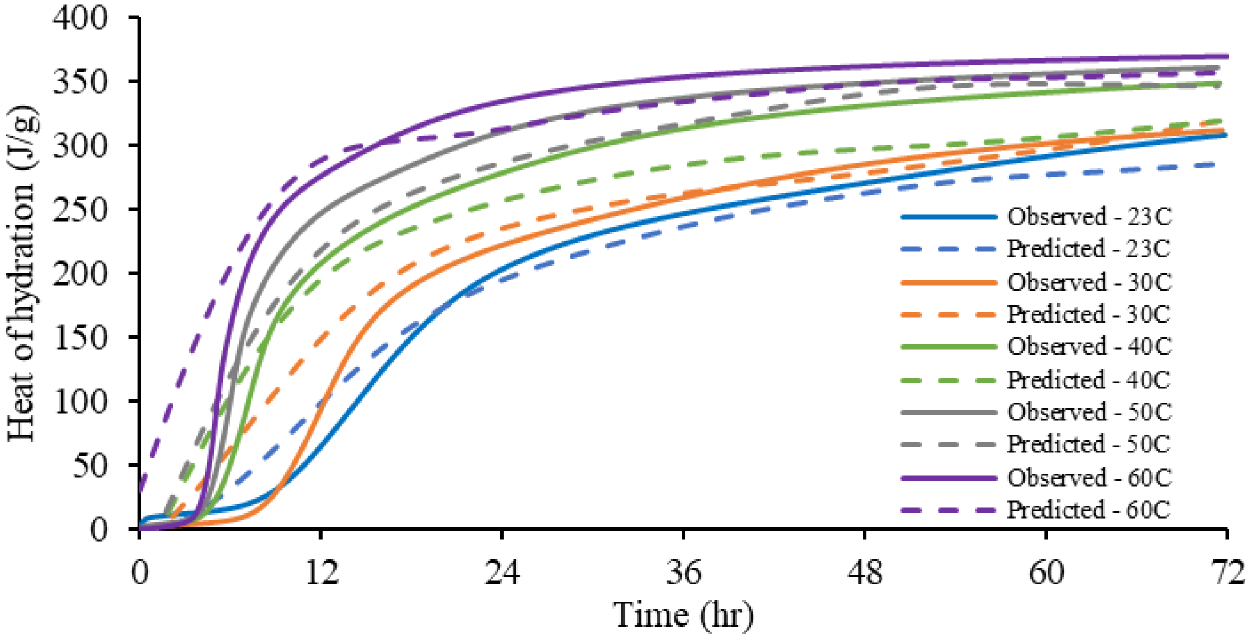
# How do we use these results?

| | OPC | Class F fly ash |
|---|---|---|
| **Oxide analysis – mass %** | | |
| MgO | 1.70 | - |
| $SO_3$ | 3.30 | - |
| $Na_2O_{eq}$ | 0.48 | - |
| CaO | - | 6.99 |
| **Phase composition – mass %** | | |
| $C_3S$ | 59 | - |
| $C_2S$ | 12 | - |
| $C_3A$ | 7 | - |
| $C_4AF$ | 10 | - |
| **Fineness ($m^2$/kg)** | | |
| SSA | - | 338.9 |
| Blaine | 391 | - |



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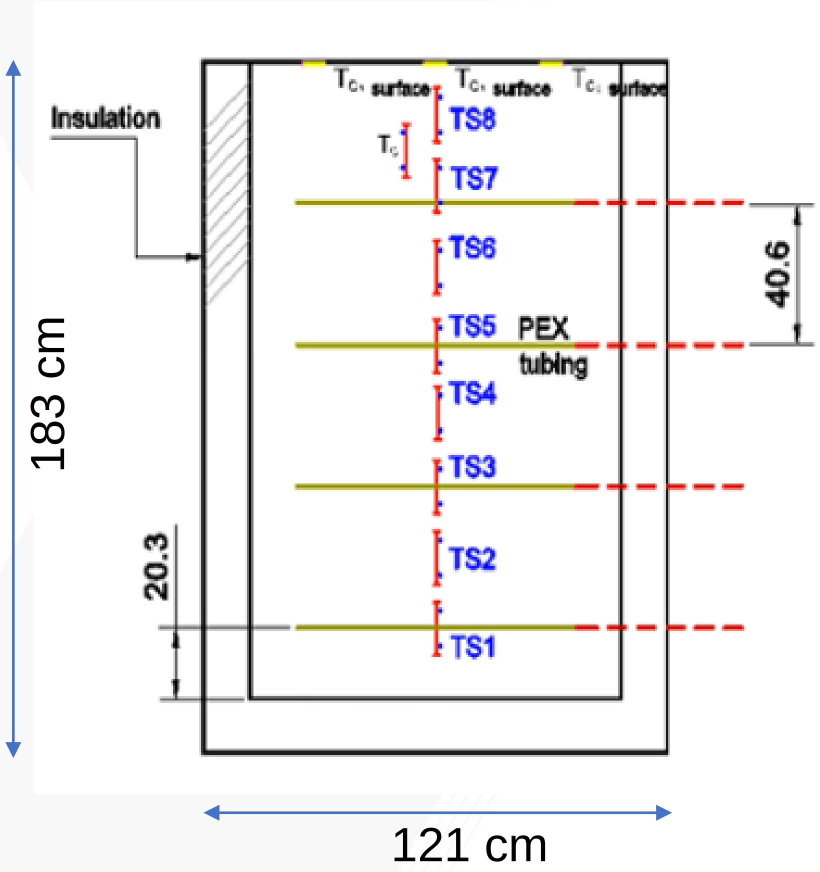


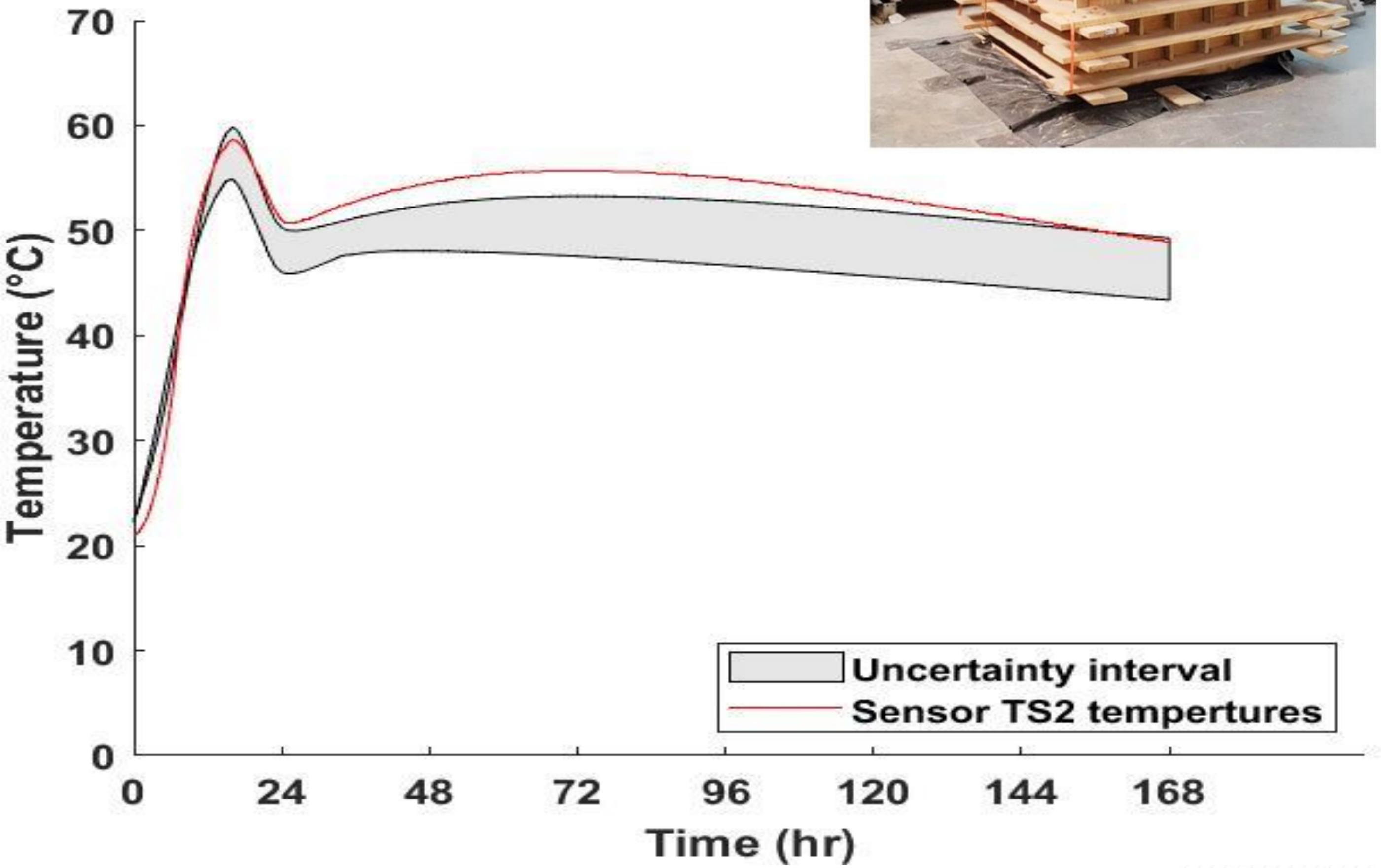


# Thank you for listening…

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