

# Numerical Models for Quantifying Degree of Hydration in Concrete Mixes with Reduced CO<sub>2</sub> Footprint

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# Environmental Concerns



A major focus of the construction industry

- CO<sub>2</sub> footprint
- Energy emissions
- Raw materials
  
- Ireland: CEM II: 80% of total cement production
- GGBS: Widely used as a mixer addition

# Motivation

To understand hydration behaviour, especially at early ages

- Influence on early-age performance of concrete
- Prevent excessive thermal gradients
- Predict long term concrete properties (e.g. diffusivity) through characterisation of pore structure

# Hydration

$$\text{Degree of hydration } (\langle) = \frac{\text{quantity of hydrated cement grains}}{\text{original quantity of cement grains}}$$

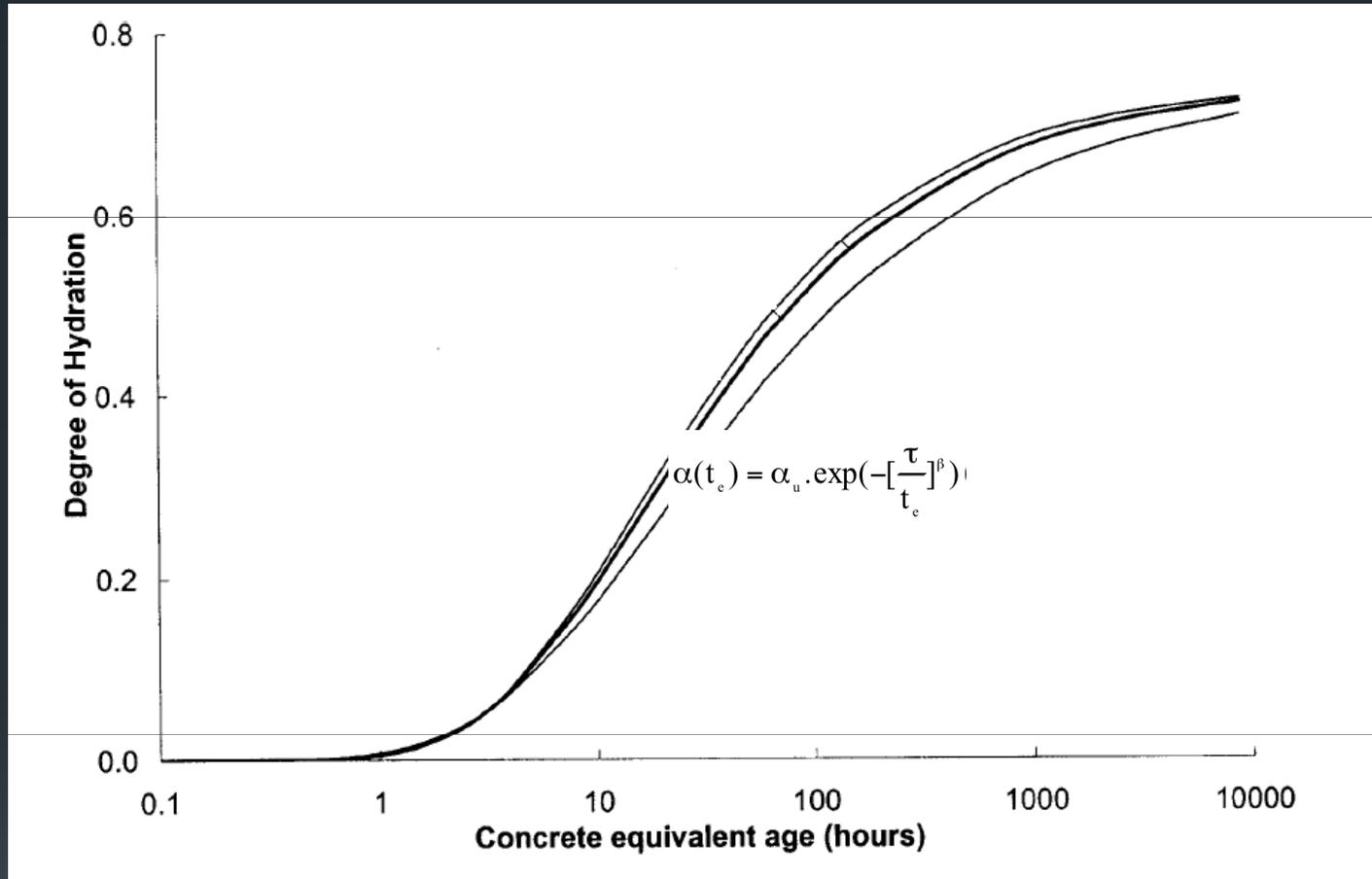
A measure of concrete maturity

- Direct quantification
  - Measure the quantity of cement gel formed
- Indirect quantification
  - Based on amount of chemically bound water or total heat generated

# Objectives

- To model the heat of hydration generated in concrete mixes manufactured using CEM II with GGBS
- To investigate key parameters
  - Age
  - Curing regime
- To quantify these effects
  - Equivalent age maturity methods
  - Temperature sensitivity calculations

# Hydration Modeling



- S-shaped hydration curves
- Exponential function:

$$\alpha(t_e) = \alpha_u \cdot \exp(-[\frac{\tau}{t_e}]^\beta)$$

# Hydration Modeling

$$\alpha(t_e) = \alpha_u \cdot \exp\left(-\left[\frac{\tau}{t_e}\right]^\beta\right)$$

$t_e$ : equivalent age at the reference temperature ( $T_r$ )

$\alpha_u$ : ultimate degree of hydration

$\tau$ : hydration shape parameter

$\beta$ : hydration time parameter (hours)

Hydration curve parameters ( $\alpha_u$ ,  $\tau$ ,  $\beta$ ) characterize generated heat for each mix

- $\beta$ : relevant to the timing of the accelerating part
- $\tau$ : represents the rate of hydration
- $\alpha_u$ : final achievable degree of hydration

# Experimental Study

- Mix parameters
  - 320 kg/m<sup>3</sup> CEM II/A-L binder
  - Target w/c ratio 0.55
  - GGBS replacement levels: 0%, 30%, 50% & 70%
  - Embedded thermocouples
  - Temperature monitoring for 1 week
  - 2cm insulation to minimize heat loss
- Temperature profiles used to quantify heat of hydration
- Numerical model with multivariate non-linear regression

# Degree of Hydration

$$\alpha_t = \frac{\text{Cumulative amount of heat evolved by the time } t}{\text{Total heat corresponding to 100\% hydration}}$$

Two key tasks:

- Measure the cumulative released heat of hydration ( $H(t)$ )
- Determine the total heat of hydration of the mix ( $H_T$ )

# Ultimate Heat of Hydration

- Particular heat associated with each cementitious phase ( $C_3S$ ,  $C_2S$ ,  $C_3A$  etc)
- XRF analysis of cements
- Application of Bogue equations

$$H_{cem} = 500 p_{C_3S} + 260 p_{C_2S} + 866 p_{C_3A} + \dots$$

- Total heat of hydration of the cementitious system:

$$H_u = H_{cem} p_{cem} + 461 p_{slag}$$

- Ultimate heat of hydration ( $J/m^3$ ) assuming 100% hydration

$$H_T = H_u c_c$$

# Evolving Heat of Hydration

- Hydration – heat generated within concrete

$$\frac{dH}{dt} = \frac{dT}{dt} \rho c_p$$

- Specific heat ( $c_p$ ): highly influenced by unbound water
- Not constant for early-age concrete

$$c_p = \frac{1}{\rho} (W_c \cdot \alpha \cdot c_{cef} + W_c \cdot (1 - \alpha) \cdot c_c + W_a \cdot c_a + W_w \cdot c_w)$$

$$c_{cef} = 8.4 T_c + 339$$

# Evolving Heat of Hydration

- Heat loss to environment
- Heat lost (assuming 1-D heat transfer):

$$-Q = \rho c A \frac{d(T_c - T_{amb})}{dt} \delta x$$

- Degree of hydration can then be calculated

# Hydration Curves

$$\alpha(t_e) = \alpha_u \cdot \exp\left(-\left[\frac{\tau}{t_e}\right]^\beta\right)$$

- Corresponding values of  $t_e$  (equivalent time) are required
- $t_e$  represents the equivalent age of a specimen cured at the reference temperature ( $T_r$ )
- Convert actual age to equivalent curing age ( $t_e$ ) using:

$$t_e(T_r) = \sum_0^t \exp\left(\frac{E}{R} \left(\frac{1}{273 + T_r} - \frac{1}{273 + T_c}\right)\right) \cdot \Delta t$$

# Hydration Curves

- E: Activation energy
- Calculated using Schindler (2005)

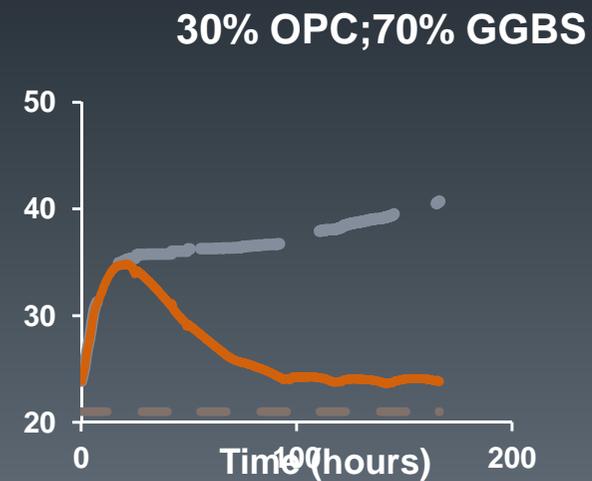
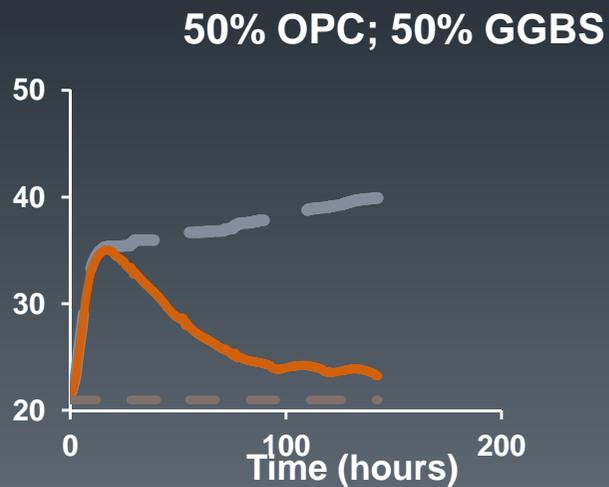
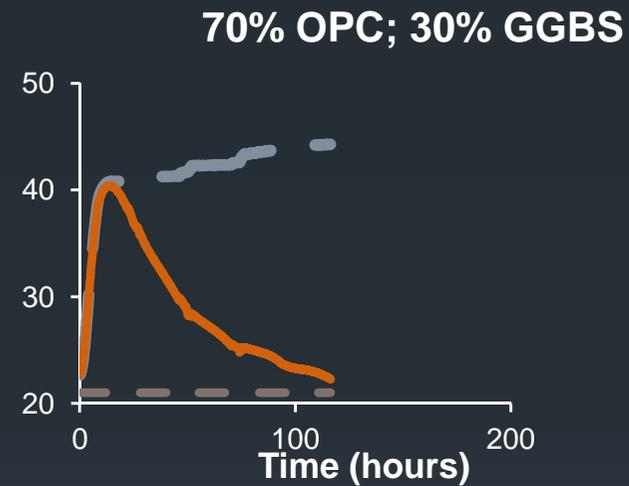
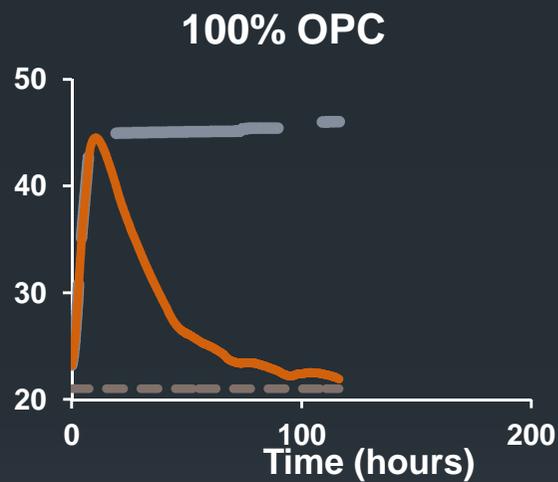
$$E = 22,100 f_E (p_{C3A})^{0.3} (p_{C4AF})^{0.25} \text{ Blaine}^{0.35}$$

$$f_E = 1 + 0.4 p_{\text{slag}}$$

- $f_E$ : activation energy modification factor for GGBS

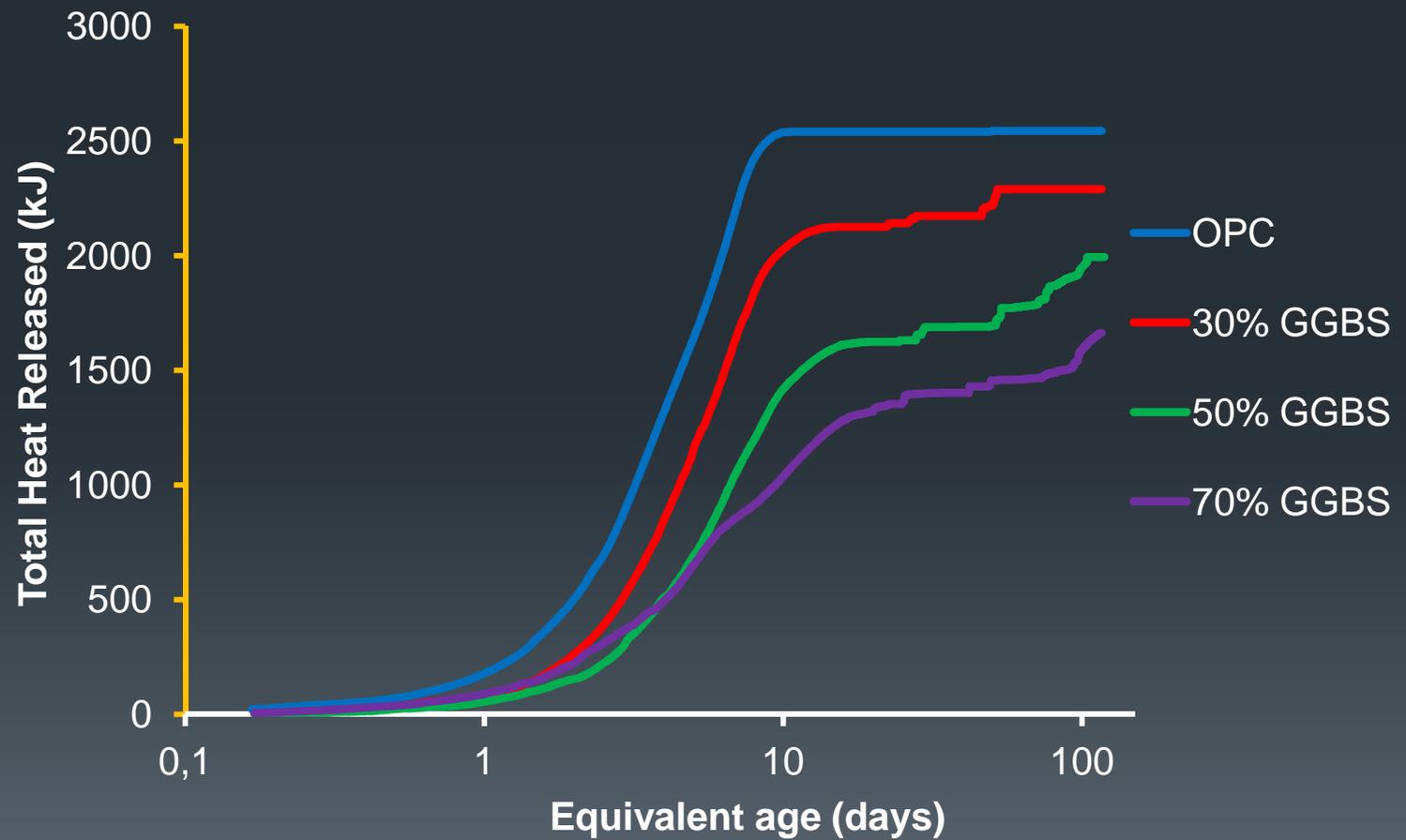
# Results

- Time-temperature profiles for each mix



# Results

- Heat evolution trends



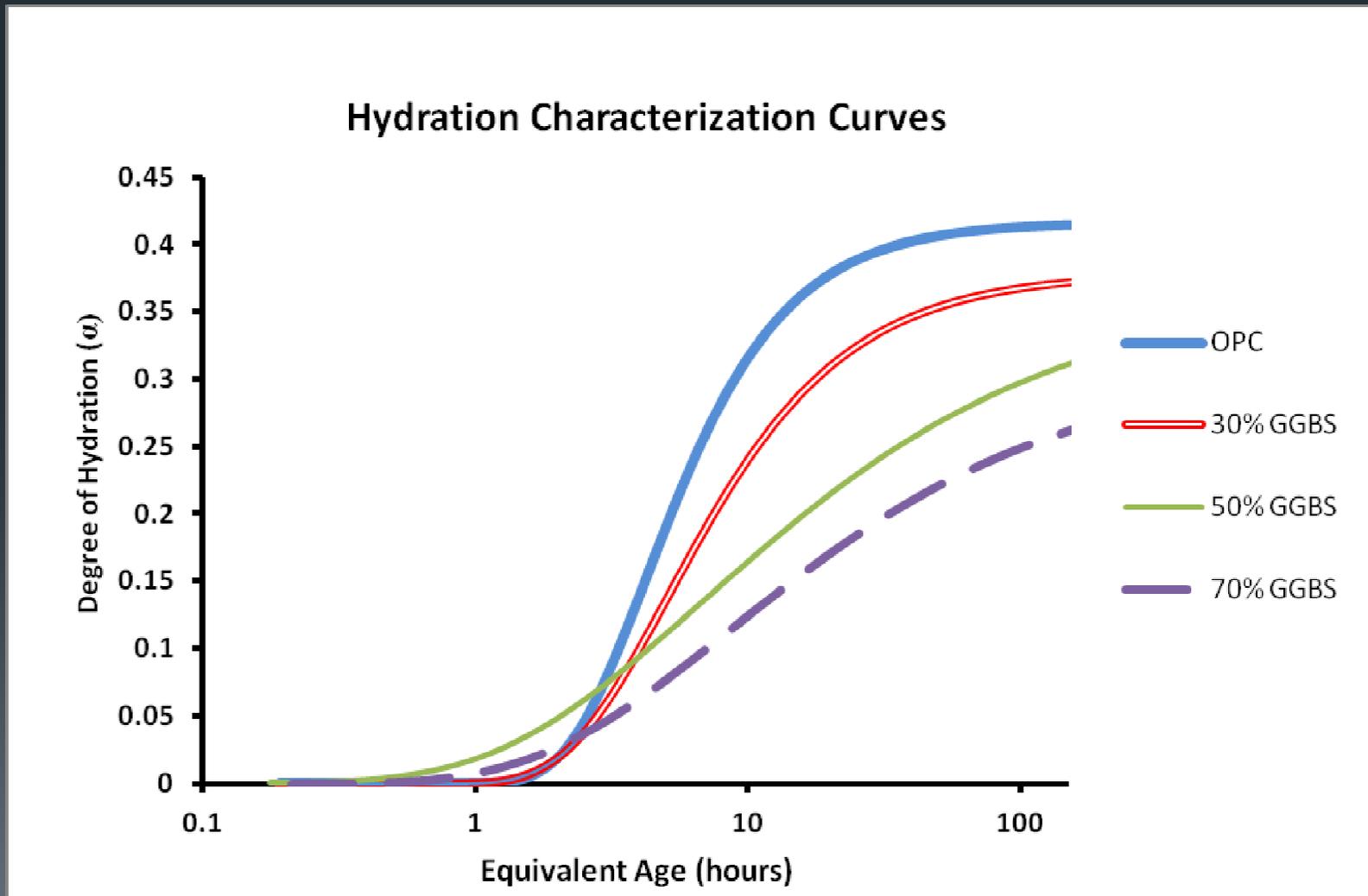
# Results

- Hydration parameters determined from multivariate regression analysis

Mix Description	$E$ (J/mol)	$H_u$ (J/g)	$\alpha_u$	$\tau$	$\beta$
CEM II	45 105	475	0.417	4.266	1.503
CEM II + 30% GGBS	50 518	470	0.378	5.101	1.1670
CEM II + 50% GGBS	54 127	468	0.369	6.906	0.575
CEM II + 70% GGBS	57 735	465	0.312	8.714	0.606

# Results

- S-shaped hydration curves based on hydration parameters



# Conclusions

Increasing GGBS content:

- Delays acceleration stage, and increases the hydration time parameter  $\alpha$
- Slows hydration rate, reduces rate parameter  $\tau$
- Requires longer term temperature monitoring
  
- Comparison with literature: behaviour is quite different than similar testing using CEM I - further research required
- Future tie-in with durability parameters

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