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Predicting Mortar Compressive Strength Using HYDCEM

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Predicting mortar compressive strength using HYDCEM

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ABSTRACT: The compressive strength of mortar is a significant property that will influence its performance in concrete or masonry. Being able to accurately model and predict the mortar compressive strength would be of great benefit to suppliers and end users alike that could possibly reduce the need for multiple physical testing. A section of the original HYDCEM cement hydration model (amoungst others) has been partitioned to focus on predicting the compressive strength of Portland cement and cement-limestone mortars, entitled HYDCEM_CompressiveStrength. The model uses the cement/binder oxide composition along with other inputs to predict the compressive strength development over time.

This paper presents a study into how accurately the HYDCEM_CompressiveStrength model can predict the mortar's compressive strength over time for European cements. Experimental results of mortar cube's and bar's compressive strength in accordance with ASTM C 109 for a CEM I + 10% limestone binder and EN196-1 for a CEM I and CEM II cement are presented along with predictions from the model following a parametric study. Comparisons have shown reasonably good agreement between measured and predicted values over time.

KEY WORDS: HYDCEM; Compressive strength; Cement; Limestone; Hydration.

1 INTRODUCTION

The compressive strength of mortar (cement and sand mixture) has a significant effect on the concrete or masonry it is added to. The ability to predict the mortar strength would therefore be very advantageous to the manufacturer and end user. This could provide useful insights into the end products performance in use, saving both time and money.

Mortar compressive strength is typically assessed using multiple cubes (50x50x50mm) or bars (160x40x40mm) cast using a specific sand, mortar mixer and cured to a specific temperature that are loaded to failure in accordance with ASTM C 109 [1] or EN 196-1 [2] that are commonly used in the United States and Europe respectively.

A number of researchers, summarised in [3], have developed empirical mathematical models to predict the compressive strength based on the cement particle size distribution or the fineness. In the United States, the compressive strength of 50x50x50mm mortar cubes in accordance with ASTM C 109 [1] has been predicted [3] using the Powers and Brownyard [4] approach. While these predictions yielded reasonable accuracy with measured compressive strengths following some calibration, it was focused on using US based cements. These predictions were undertaken using the CEMHYD3D cement hydration model [3] that used pixelated images of cement slices that followed a cellular atomia approach to model ongoing hydration. To date, there have been no attempts to use a similar approach to predict mortar compressive strengths on European cements, in accordance with EN197-1 [5].

The HYDCEM cement hydration model, previously written in MATLAB [6], has been recently re-written in C# to improve functionality for advanced analysis including thermodynamic studies. A number of selected sub-models from the original, including one for mortar compressive strength predictions, have been excluded from the latest version. These are now available as individual MATLAB models to undertake specific analysis. The HYDCEM_CompressiveStrength model predicts the mortar's compressive strength development over time employing the Powers and Brownyard approach using the cement's chemical oxide compositions, w/c ratio and temperature for Portland cement and limestone binders.

This paper presents comparisons between the measured and predicted compressive strengths of EN197-1 [5] Portland cement and limestone binders over time from ASTM C 109 cubes [1]. The results show that reasonable comparisons can be made over 28-days following calibration.

2 POWERS GEL-SPACE MODEL

The original Powers and Brownyard model [4] to predict the compressive strength of cement-sand mortars was developed in 1948 and modified by Powers in 1958 [7]. The model relates the mortar compressive strength to the gel to space ratio, which is described as the proportion of gel volume to the volume of capillary porosity, as described in Figure 1 as predicted by [4].

This is described mathematically in Equation 1, where X is the gel-space ratio and α is the degree of hydration. The authors were the first to introduce the degree of hydration concept to compressive strength by using Equation 2 where $\alpha_c(t)$ is the mortar compressive strength over time, σ_A is the intrinsic cement strength and n is a dimensionless parameter (2.6 to 3.0).

The intrinsic strength is taken as the compressive strength measurement at 3-days and used to predict the 7 and 28-day strengths thereafter. The intrinsic strength is lower for cements with higher (> 7%) C_3A contents.

$$X = \frac{0.68\alpha}{0.32\alpha + \mathrm{w/c}} \quad (1)$$

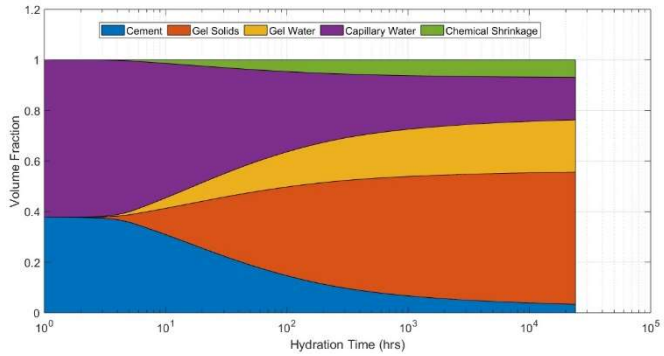

Figure 1 Change in volume with ongoing hydration [4,6].

$$\sigma_c(t) = \sigma_A X(t)^n \tag{2}$$

2.1 Previous Modelling Work

CEMHYD3D [3] is a three-dimensional cement hydration model written in C to simulate Portland cement hydration and microstructure development. CEMHYD3D employs the discrete or pixel approach with digitised colour images to represent the cement under investigation and the cellular-automata method where the microstructure is represented as a grid of discrete three-dimensional cubic elements. Each volume-pixels, or 'voxels' represents an anhydrous or hydrate phase or pore. Bentz [3] used intrinsic strength values of 129 and 99MPa for NIST Cements 115 and 116 respectively (Figure 2) with a w/c ratio of 0.485 along with CEMHYD3D that provided good correlations between measured and predicted, as shown in Figure 3.

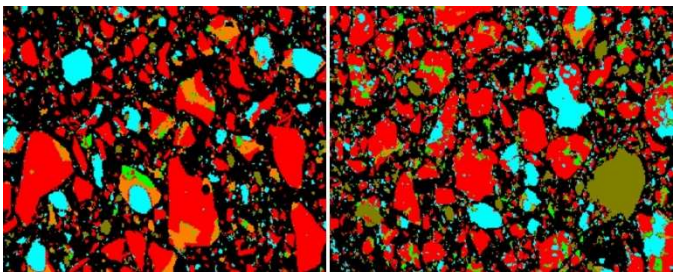

Figure 2 NIST cements 115 & 116

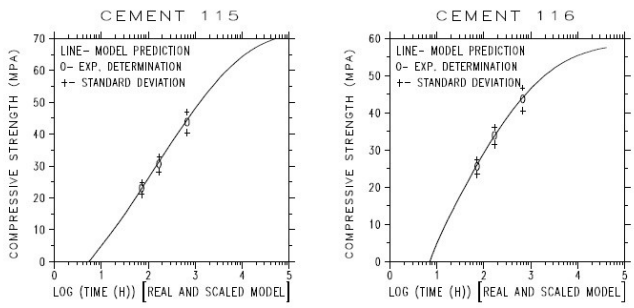

Figure 3 Predicted and measured compressive strengths for NIST Cements 115 and 116 [3]

3 HYDCEM

3.1 Model design

The HYDCEM_CompressiveStrength model provides predictions of mortar compressive strengths over a 28-day period in 1hr timesteps. The model calls a number of bespoke functions from the main script to undertake the analysis using data input via an Excel spreadsheet (input.xlsx), divided into multiple tabs, by the user. All data is described along with their numerical information, to aid the user's understanding. The input data required by HYDCEM_CompressiveStrength model include the w/c ratio, % Limestone, curing temperature, element molar masses, intrinsic strength (MPa) and non-dimensional n factor, cement and limestone (on separate tabs) oxide compositions. The input file also includes the information required to determine the individual cement phase and overall degree of hydration (α), required for Equation 1.

The dissolution of the four cement clinker phases in HYDCEM_CompressiveStrength is simulated using a function following the approach developed by Parrot and Killoh [8]. The degree of hydration over time of each phase is calculated using a suite of empirical expressions. All Constants (K, N, H) and properties (activation energies, Blaine surface area, etc.) required are changeable by the user in the input file.

The dissolution of each clinker phase is determined using Equations (3)-(5) which represent nucleation and growth, diffusion and formation of a hydration shell respectively with the lowest hydration rate R_t taken as the rate-controlling value. The degree of hydration (α) is expressed in Equation 6. The K, N and H values used for the three phases are those proposed by Lothenbach *et al.* [9-11]. The influence of the surface area on the initial hydration is included, as well as the influence of w/c (Equation 7). The overall degree of hydration is calculated based on the weighting of the four cement phases, namely C_3S, C_2S, C_3A and C_4AF using a modified Bogue method. The input used is summarised in Table 1 below.

$$R_t = \frac{K}{N}(1-\alpha_t)\left(-ln(1-\alpha_t)\right)^{(1-N)} \tag{3}$$

$$R_t = \frac{K(1-\alpha_t)^{\frac{2}{3}}}{1-(1-\alpha_t)^{\frac{1}{3}}} \tag{4}$$

$$R_t = K(1-\alpha_t)^N \tag{5}$$

$$\alpha_t = \alpha_t - 1 + \Delta_t \cdot R_t - 1. \tag{6}$$

$$f(w/c) = (1 + 3.333 * (H * w/c - \alpha_t))^4; \text{ for } \alpha_t > H * w/c \tag{7}$$

Much has been written about the appropriateness of nucleation and growth, diffusion or the formation of a hydration shell to predict cement dissolution. Dissolution theory is providing theoretical and experimental evidence to suggest the most accurate way of describing the early dissolution of cement. However, the Parrot and Killoh method has also been shown to give good comparisons with experimental results, despite being an empirical method. Until the dissolution theory is developed to a point where numerical predictions are possible, the Parrot and Killoh method will

Table 1 Parameters used in the Parrot and Killoh degree of hydration analysis

Parameter	C_3S	C_2S	C_3A	C_4AF
K[1]	1.5	0.5	1	0.37
N[1]	0.7	1	0.85	0.7
H[1]	1.8	1.35	1.6	1.45
K[2]	1.1	0.7	1	0.4
N[2]	3.3	5	3.2	3.7
K[3]	0.05	0.02	0.04	0.015
Apparent activation energy (J/mol)	41,570	20,785	54,040	34,087

[1] Nucleation & growth; [2] Shell formation; [3] Diffusion

continue to be employed in HYDCEM_CompressiveStrength.

4 EXPERIMENTAL WORK AND RESULTS

4.1 Testing

For this study, nine mortar cubes per cementitious mix (Table 2) were prepared for compressive strength testing at 3, 7 and 28-days in accordance with ASTM C 109 [1]. All samples regardless of cement or limestone proportion are made with a w/c or w/b ratio of 0.485 and a silica sand:cement ratio of 2.75 as per the standard. The mortar was mixed in a paddle mixer and placed into nine 50x50x50mm cubes and compacted using a virating table. The samples and moulds were placed inside sealed plastic bags for 24hrs after which the mortar cubes were carefully removed and cured in a water bath at 20 ± 2°C until testing. At the appropriate time, three cubes were removed from the water bath, dried and placed into the compression apparatus.

Table 2 Mix proportions

Mix ID	Mass of Ingredients (g)				
	Cement	LS	Sand	Water	GGBS
CEM I	888	0	2442	431	0
CEM I + 5% LS	843	45	2442	431	0
CEM I + 10% LS	799	89	2442	431	0
CEM I + 15% LS	755	133	2442	431	0
CEM II	888	0	2442	431	0
CEM I + 50% GGBS	444	0	2442	431	444

4.2 Cement and limestone properties

The properties of the Portland cement and limestone used for the mortars are described in Table 3 in terms of their oxide contents using XRF analysis as required by the model. Figure 4 shows the location of this cement and possible solids that may form on CaO-SiO_2-Al_2O_3 and C_3A-$CaSO_4$-$CaCO_3$ Ternary diagrams determined using another HYDCEM MATLAB model (HYDCEM_Ternary). Ternary diagrams can provide graphical representation of more advanced thermodynamic predictions. The CaO-SiO_2-Al_2O_3 diagram provides the relationships between the predicted phases in systems

Table 3 Oxide proportions for the cements and limestone

Oxide (g/100g)	CEM I	CEM II	Limestone
SiO_2	19.04	17.5	4.54
Al_2O_3	5.01	4.6	1.07
Fe_2O_3	2.83	2.6	0.73
CaO	63.4	62	54.5
MgO	2.31	2.3	1.96
Na_2O	0.28	0.26	0.01
K_2O	0.54	0.5	
CaO_free	1.71	1.62	
CO_2	2.20	6.27	36.70
SO_3	2.65	2.45	
Soluble Na_2O	0.14		0.01
Soluble K_2O	0.43		0.13
MgO periclase	1.00	1.00	

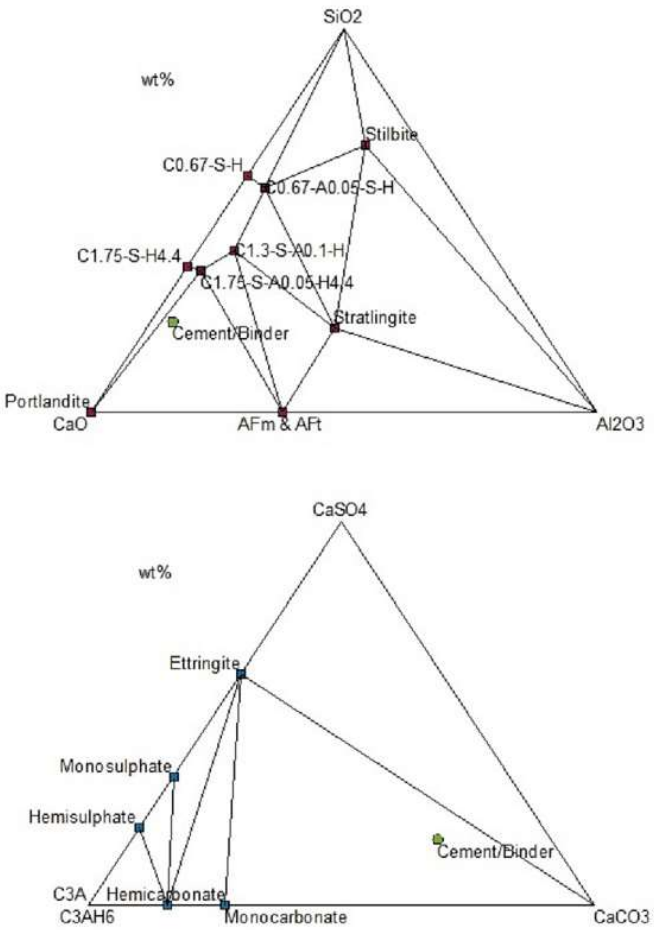

Figure 4 Ternary diagrams - CEM I + 10% Limestone binder

undersaturated in $Ca(OH)_2$, AFm and Aft [12]. For over undersaturated systems, framework silicates in the form of stilbite will precipitate [12]. The C_3A-$CaSO_4$-$CaCO_3$ diagram shows the relationships for the carbonate- and sulfate-bearing phases. A typical Portland cement with no limestone will consist of monosulfate, ettringite and hemicarbonate, C-S-H and Portlandite [12]. Using a modified Bogue function written into the model, the C3S, C2S, C3A and C4AF cement phase proportions were 50.59%, 11.19%, 7.67% and 7.84%

respectively. While each of the mixes in Table 2 were cast, due to COVID-19, only the CEM II mix with a 10% limestone content was tested.

4.3 Results

The compressive strength results at 3, 7 and 28-days for Mix CEM I + 10% limestone are presented in Table 4. As shown, there is an expected increase in compression strength up to 7 days, which, albeit at a slower rate, increases to 28 days.

The addition of limestone stabilises ettringite that increases the total volume of hydration products due to its low density. The resulting decrease in porosity leads to higher compressive strengths, especially for limestone replacement levels in the range 5-10% [9]. Beyond 10%, a loss in compressive strength has been reported in the literature [13-15]. The fineness of limestone can also affect the compressive strength as shown by calorimetry measurements [9] as it accelerates the rate of hydration as it provides additional surface for the nucleation and growth of hydration products [16,17].

5 PREDICTION OF ASTM C 109 COMPRESSIVE STRENGTH

In order to get a good fit between the measured and predicted compressive strengths, a parametric study was undertaken by varying the intrinsic strength and n parameter. The result of varying these properties are shown in Figure 5 which varied the value of n while keeping the intrinsic strength constant and *vice versa* respectively. The oxide contents were those shown in Table 3 with a w/c ratio of 0.5 and temperature of 20°C. As may be shown that, varying the n value while maintaining the intrinsic strength at 82MPa, leads to a nonlinear variation of the compressive strength over time. In contrast, varying the intrinsic strength while keeping the n value at 2.5 gives a linear change in compressive strength over time (Figure 5).

As the 3-day compressive strength was found to be 19MPa (Table 4), it was decided to run an analysis with an intrinsic strength and n value of 100MPa and 2.4 respectively. This was found to give a reasonable prediction of the measured strengths, especially over time, as shown in Figure 6. At 3 days, there is a slight difference between the two sets of results that reduces over time. This is similar to the values used by Bentz [3] who used an n value of 2.6 and 129 & 99MPa for the intrinsic strength for the 115 and 116 cements respectively.

As the C_3A phase proportion for the cement (7.67%) is greater than 7%, the intrinsic strength here is lower than that used (on average) than cements 115 and 116 (here 100MPa).

Table 4. Compressive strength results

Time (days)	3	7	28
Compressive strength (MPa)	19	37	49

6 PREDICTION OF EN196-1 COMPRESSIVE STRENGTH

As the original experimental work was cut short due to COVID-19, it was decided to investigate the accuracy of the Powers gel-space method to predict the compressive strength of 160x40x40mm mortar samples made to EN196-1. Using a set of results (Table 5) for a CEM I and CEM II cement (Blaine fineness = 386m^2/kg and 474 m^2/kg respectively) provided by a leading cement manufacturer, the procedure in Section 5 was repeated. The Ternary diagram description of these cements is shown in Figure 7 and Figure 8. The cement phase proportions

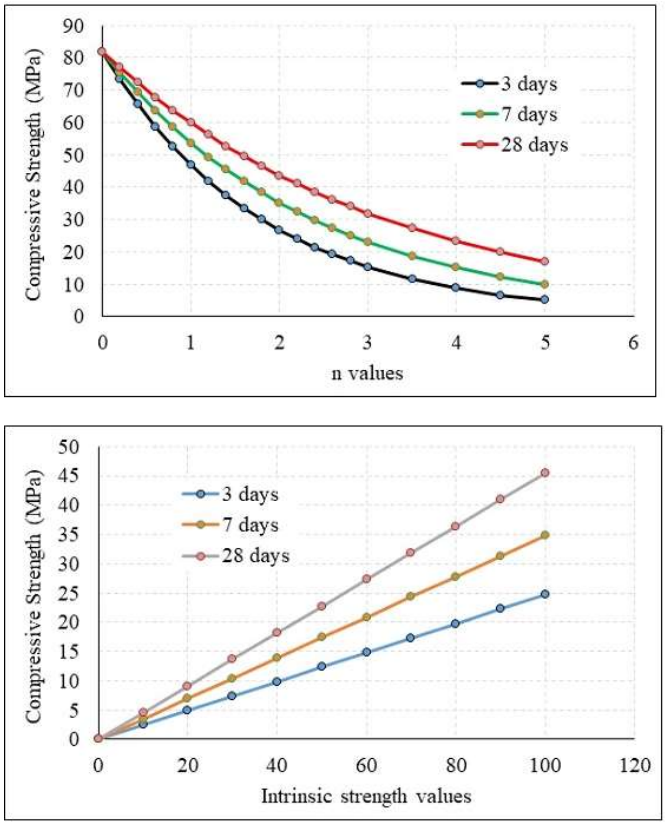

Figure 5 Parametric study results with varying n and σ_A

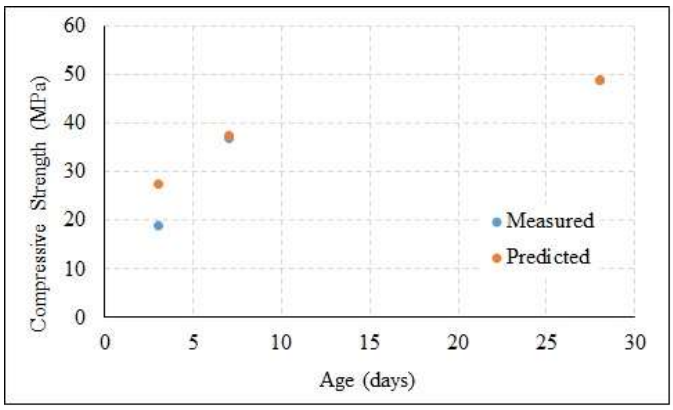

Figure 6 Predicted and measured compressive strength

Table 5 EN196-1 Compressive strength results

Time (days)	2	7	28
CEM I Compressive strength (MPa)	30.7	48.1	62.4
CEM II Compressive strength (MPa)	31	46.7	58.4

(C_3S, C_2S, C_3A & C_4AF) were calculated from the oxide compositions in Table 3 to be 57.35%, 11.32%, 8.49% and 8.61% for the CEM I and 45.69, 15.70, 7.79 and 7.91 for the CEM II cement using the modified Bogue function in the model.

Using the previous parametric study, the measures and predicted compressive strength comparisons for the CEM I and CEM II cements are shown in Figure 9 and Figure 10. Again, as shown previously, the 2-day comparisons are slightly different and improve over time. Despite this, there is very

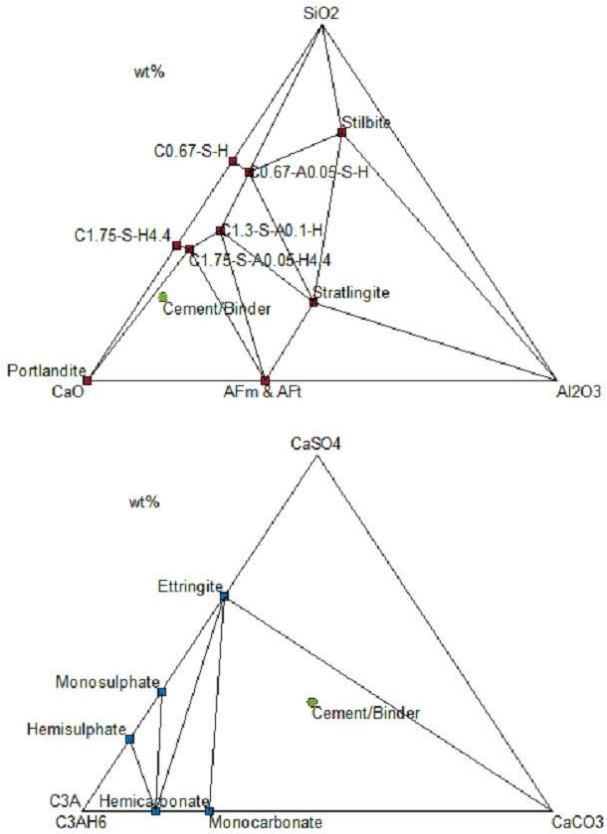

Figure 7 Ternary diagrams for CEM I cement

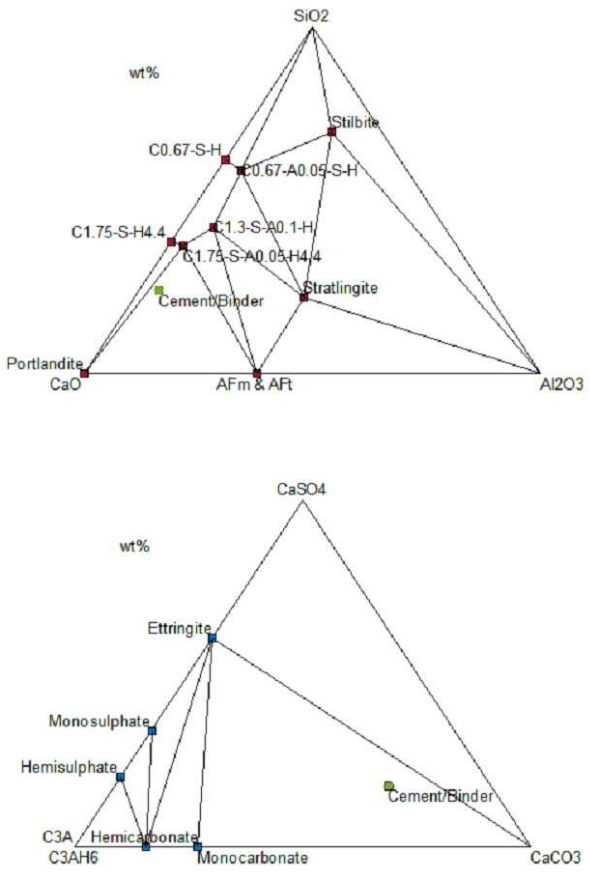

Figure 8 Ternary diagrams for CEM II cement

good agreement between the predicted and measured compression strengths using EN196-1.

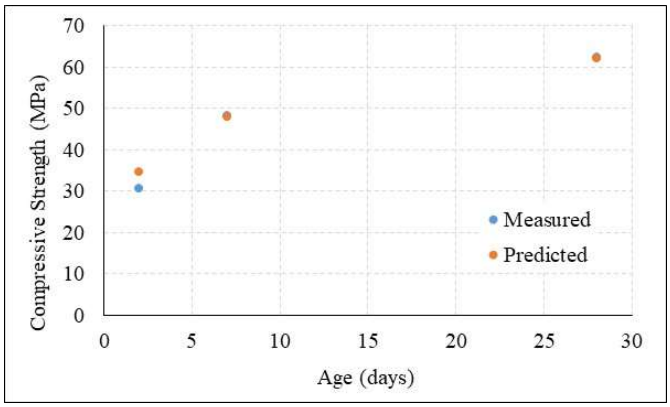

Figure 9 Predicted and measured compressive strengths for the CEM I cement testing to EN196-1

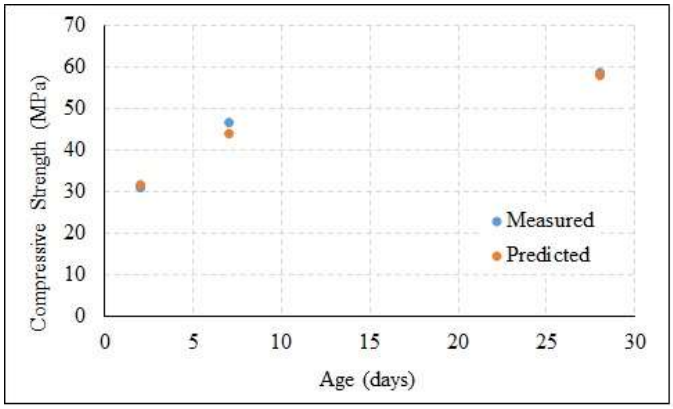

Figure 10 Predicted and measured compressive strengths for the CEM II cement testing to EN196-1

7 CONCLUSION

The HYDCEM_CompressiveStrength MATLAB model has be shown to give reasonably accurate predictions of the compressive strength over time for CEM I and CEM I + Limestone cements as measured using EN196-1 and ASTM C 109 respectively. By using appropriate intrinsic strength and n values, reasonable predictions can be achieved, particularly over time. The model employs the Powers 'gel-space and Parrot and Killoh methods to derive useful predictions using appropriate data input.

The results here are somewhat limited (due to the COVID-19 pandemic) so more predictions need to be performed but initial analysis looks promising as a means to predict mortar strength over time using this model.

ACKNOWLEDGMENTS

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REFERENCES

[1] ASTM C109-13. (2013). "Standard Test Method for Compressive Strength of Hydraulic Cement Mortars (Using 2-in. or [50-mm] Cube

Specimens)" Annual Book of ASTM Standards, V. 04.01, ASTM International, West Conshohocken, PA.
[2] EN 196-1: 2005 (E)., 2005. Methods of testing cement (Part 1): Determination of strength.
[3] D. P. Bentz, Three-dimensional computer simulation of cement hydration and microstructure development, J. Am. Ceram. Soc. 80 (1) (1997) 3–21.
[4] T.C. Powers, T.L. Brownyard, Studies of the Physical Properties of Hardened Portland Cement Paste, ACI Journal, Proceedings V. 43, Oct. 1946 to Apr. 1947 (published in multiple parts); also published as PCA Bulletin 22, Research Laboratories of the Portland Cement Association, Chicago, IL, 1948.
[5] BS EN 197-1:2000, Cement — Part 1: Composition, specifications and conformity criteria for common cements
[6] N. Holmes, D. Kelliher, M. Tyrer, Simulating cement hydration using HYDCEM, Construction and Building Materials, Volume 239, (2020)
[7] T. C. Powers, Structure and Physical Properties of Hardened Portland Cement Paste, Research and Development Laboratories of the Portland Cement Association, Research Department Bulletin 94, J. Am. Ceram. Soc. Vol 41, (1958)
[8] L.J. Parrot, D.C. Killoh, Prediction of cement hydration, Br. Ceram. Proc., 35 (1984), pp. 41-53
[9] Lothenbach, B., Le Saout, G., Gallucci, E. and Scrivener, K. (2008) Influence of limestone on the hydration of Portland cements, Cement and Concrete Research 38 pp. 848–860.
[10] Lothenbach, B., Winnefeld, F., Alder, C., Wieland, E., and Lunk, P. (2007) Effect of temperature on the pore solution, microstructure and hydration products of Portland cement pastes, Cement and Concrete Research 37 (4) pp. 483–491.
[11] Lothenbach, B. Thermodynamic modelling of the effect of temperature on the hydration of Portland cement, International RILEM Symposium on Concrete Modelling – CONMOD 2008, 26-28 May, Delft, The Netherlands.
[12] Scrivener, K., Snellings, R. and Lothenbach, B. eds., 2016. A practical guide to microstructural analysis of cementitious materials (Vol. 540). Boca Raton: Crc Press.
[13] T. Schmidt, Sulfate attack and the role of internal carbonate on the formation of thaumasite. Thesis EPFL, Lausanne, Switzerland, 2007.
[14] S. Tsivilis, J. Tsantilas, G. Kakali, E. Chaniotakis, Sakellariou, The permeability of Portland limestone cement concrete, Cem. Concr. Res. 33 (2003) 1465–1471.
[15] T. Vuk, V. Tinta, R. Gabrovšek, V. Kaucic, The effects of limestoneaddition, clinker type and fineness
[16] J. Stark, Optimierte Bindemittelsysteme für die Betonindustrie, Beton 54 (10) (2004) 486–490.
[17] J. Pera, S. Husson, B. Guilhot, Influence of finely ground limestone on cement hydration, Cem. Conc. Comp. 21 (2) (1999) 99–105.