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Prediction model for the hydration properties of concrete

Inyeop Chu[1a], Muhammad Nasir Amin[2b] and Jin-Keun Kim[*3]

[1]*Civil Engineering Team, Samsung Engineering Co. Ltd., Seoul, Korea*
[2]*Civil Engineering Dept., National University of Science and Technology, Islamabad, Pakistan*
[3]*Civil and Environmental Engineering Department,*
Korea Advanced Institute of Science & Technology, Daejeon, Korea

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Abstract. This paper investigates prediction models estimating the hydration properties of concrete, such as the compressive strength, the splitting tensile strength, the elastic modulus,and the autogenous shrinkage. A prediction model is suggested on the basis of an equation that is formulated to predict the compressive strength. Based on the assumption that the apparent activation energy is a characteristic property of concrete, a prediction model for the compressive strength is applied to hydration-related properties. The hydration properties predicted by the model are compared with experimental results, and it is concluded that the prediction model properly estimates the splitting tensile strength, elastic modulus, and autogenous shrinkage as well as the compressive strength of concrete.

Keywords: temperature; aging; hydration properties; apparent activation energy; prediction model

1. Introduction

Concrete is an aging material, and the hydration-related properties of concrete change with time. Meanwhile, the heat of hydration in mass concrete structures creates a temperature gradient between the inner and surface. This temperature gradient affects the properties of the concrete, i.e., the compressive strength, elastic modulus, splitting tensile strength, and autogenous shrinkage. Also, the temperature variations caused by cold-weather or hot-weather conditions have the same influence on concrete. Hydration properties such as the compressive strength, elastic modulus, splitting tensile strength, and autogenous shrinkage are factors that must be considered in the design and construction of concrete structures. Specifically, an evaluation of the thermal cracking of a mass concrete structure requires an estimation of the elastic modulus and tensile strength of early-age concrete with the temperature. Therefore, it is very important to estimate the properties of concrete according to different temperature and aging factors (Abdel-Jawad 2006, Alexander and Taplin 1962, Freiesleben Hansen and Pedersen 1977, Gardner 1990, Kim *et al*. 1998, Kjellsen and Detwiler 1993, Lew and Reichard 1978, Tian *et al*. 2013, Zhang *et al*. 2008, Zou *et al*. 2013).

Many existing evaluations of the influence of temperature and aging on the hydration

*Corresponding author, Professor, E-mail: kimjinkeun@kaist.ac.kr
[a]Assistant Professor
[b]Ph.D.

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properties focus primarily on the compressive strength, while only a few prediction models are available for estimating the elastic modulus and splitting tensile strength (Chengju 1989, Gardner 1990, Kim *et al.* 2001, Tank and Carino 1991). To evaluate the validity of a prediction model, not only the compressive strength but also other properties which are related to the hydration process should be estimated using the prediction model. Among several existing models, the model proposed by Kim *et al.* (2001), which is based on a new apparent activation energy function, was reported to overcome the shortcomings of previous prediction models.

The objectives of this study are to evaluate the validity of the prediction model which is proposed by Kim *et al.* (2001) for estimating the hydration-related properties such as the splitting tensile strength, elastic modulus, and autogenous shrinkage as well as the compressive strength of concrete.

2. Prediction model

Although the Arrhenius law is generally accepted (Freiesleben Hansen and Pedersen 1977, Han and Han 2011, Jonathan *et al*. 2011, Nielsen 2007, Viviani *et al*. 2007, Waller *et al*. 2004) as the most suitable rate function for hydration of concrete among several prediction models, several researches (Chanvillard and D'Aloia 1997, Jonasson 1985, Kjellsen and Detwiler 1993) about the shortcomings of the Arrhenius equation have been reported.

A prediction model was proposed by Kim *et al.* (2001) to estimate the compressive strength development with temperature and aging. This model mitigated the shortcomings of previous models and reasonably approximated the experimental results pertaining to the compressive strength. This paper investigates the effectiveness of this model as a tool for predicting the hydration properties like the splitting tensile strength, elastic modulus, and autogenous shrinkage as well as the compressive strength of concrete. The following equation is the prediction model proposed by Kim *et al.* (2001).

$$\frac{S}{S_u} = 1 - \frac{1}{\sqrt{1 + A\sum_{i=1}^{n}\left[e^{-\frac{E_o}{RT_i}e^{-\alpha t_i}} + e^{-\frac{E_o}{RT_i}e^{-\alpha t_{i-1}}}\right](t_i - t_{i-1})}} \tag{1}$$

where, S is the compressive strength, S_u is the limiting compressive strength, A is a constant, R is the gas constant and equal to 8.3144 J/K·mole, T_i is the curing temperature at time step i (K), E_o is the initial apparent activation energy (J/mole), α is a constant, t_{i-1} is the initial age of time step i (days) and t_i is the final age of time step i (days). This equation involves four unknown parameters, t_o, E_o, α, and A.

After the prediction model was introduced, the application of the model has been investigated by several researchers (Kim *et al.* 2002, Chu *et al.* 2012). Kim *et al.* (2002) applied the model to predict the elastic modulus and splitting tensile strength as well as the compressive strength of concrete. Reasonably good agreement was shown between the predicted results and the measured results. However, the apparent activation energy function was determined using the results of the compressive strength only. While Chu *et al*. (2012) reported that the prediction model couldalso beapplied to predict the autogenous shrinkage of concrete, there has been no attempt to apply the prediction model to as determination of all hydration-related properties (compressive strength, splitting tensile strength, elastic modulus, and autogenous shrinkage) using the same apparent activation energy.

The apparent activation energy can be interpreted from the two standpoints of a 'micro' level and a 'macro' level. At the macro-level, the apparent activation energy is related to the increasing development rate of the compressive strength. Thus, if the model is applied to other properties for which the increasing rate is different from that of the compressive strength, the regression curves will have different levels of apparent activation energy according to different properties. On the other hand, the apparent activation energy at the micro-level is a function of the degree of cement hydration. Thus, if the apparent activation energy is considered as a characteristic property of concrete at the micro-level, the apparent activation energy is a constant value in all types of hydration-related properties. Many researchers (Chanvillard and D'Aloia 1997, Riding *et al*. 2011, Kada-Benameur*et al.* 2000, Kjellsen and Detwiler 1993, Wang *et al*. 2007) have proposed that the apparent activation energy is related to the hydration process of cement. Therefore, it can be assumed that the apparent activation energy is a characteristic property of concrete and that it has a constant value in all types of hydration-related properties.

The increasing rates of the splitting tensile strength, elastic modulus, and autogenous shrinkage are dissimilar to that of the compressive strength, and the dissimilarity must be considered in Eq. (1). The proportional constant A in Eq. (1) can simulate the differences in the increasing rate, even when the apparent activation energy is identical to different hydration-related properties. Therefore, it can be assumed that the difference in the increasing rate is able to be estimated by modifying the constant A with hydration-related properties. In this paper, based on the previous assumption, experimental results of hydration-related properties like the compressive strength, elastic modulus, splitting tensile strength, and autogenous shrinkage are analyzed using the prediction model, Eq. (1).

3. Experiments of hydration-related properties of concrete with temperature and aging

3.1 Experimental program

For the application of the proposed prediction model, the experimental results reported in previous research (Chu *et al*. 2012) are adopted. Table 1 shows the mix proportions used in the experiments. Ordinary Portland cement (ASTM type I) and silica fume are used as cementitious materials. The chemical composition and the physical properties of the cementitious materials are tabulated in Table 2. Crushed gravel (4~20 mm with a maximum nominal size of 20 mm), and river sand are used as coarse aggregate and fine aggregate, respectively. The respective values of specific gravity and absorption of coarse aggregate (2.58, 0.46%) and fine aggregate (2.56, 1.73%) are obtained by using ASTM C127 and ASTM C128, respectively. The fineness modulus of sand is calculated by a sieve analysis, and is equal to 0.62. Furthermore, to achieve good workability and consolidation of the concrete, different dosages of super plasticizer are used as the ratio of cementitious materials (Table 1).

In this experiment, for each mix proportion, the autogenous shrinkage under an isothermal curing condition (20, 30, and 40℃) was measured. Six identical 100 × 100 × 400 mm prism specimens, in which embedment strain gages were installed, were cast. The specimens were then divided into three groups of two specimens each so as to test all groups simultaneously but under

Table 1 Mix proportions

Mix ID	Curing temperature, (℃)	w/cm	*S/a*	Unit weight (kg/m³)					Ad^C (%)
				W	*C*	*SF*[a]	*S*	*G*[b]	
C30/7SF	20,30,40	0.30	0.40	163	505	38	665	1005	1.2
C35/7SF	20,30,40	0.35	0.40	175	465	35	665	1007	1.0
C40/5SF	20,30,40	0.40	0.39	170	404	21	671	1064	0.8
C40	20,30,40	0.40	0.39	170	425	-	671	1064	0.6

[a]Silica fume, 7% for C30/7SF and C35/7SF, while 5% for C40/5SF of total weight of cementitious materials
[b]Maximum aggregate size of 20mm
[c]Superplasticizer (ASTM Type-F high range water-reducing admixture), % of total cementitious materials

Table 2 Physical and chemical properties of cementitious materials

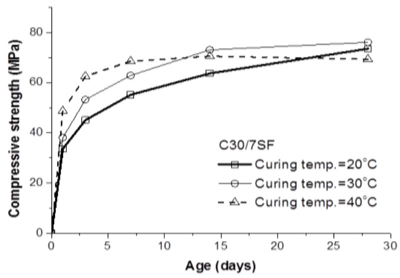
Item	Unit	OPC Type-1	Silica fume
Specific surface (Blaine)	cm^2/g	2996	191000
Specific gravity	g/cm^3	3.14	2.15
CaO	%	61.30	-
SiO_2	%	21.47	96.00
Al_2O_3	%	4.32	0.13
Fe_2O_3	%	3.34	0.05
MgO	%	2.62	0.22
Cl	%	0.01	0.01
K_2O	%	1.38	0.33
Na_2O	%	0.58	0.16
LOI	%	2.03	1.30
SO_3	%	2.09	1.04
		Compounds	
C_3S	%	45	-
C_2S	%	28	-
C_3A	%	6	-
C_4AF	%	10	-

distinct isothermal temperatures (20, 30, and 40℃). To achieve isothermal temperatures, a separate climatic chamber was used for each curing temperature. However, in all chambers, a standard humidity of 60% was maintained throughout the monitoring of experimental data. For each specimen, the corresponding isothermal temperature was strictly maintained by air cooling starting from casting of the specimen until completing the test. Details of the experimental procedure for autogenous shrinkage can be founded in previous research (Chu *et al*. 2012)

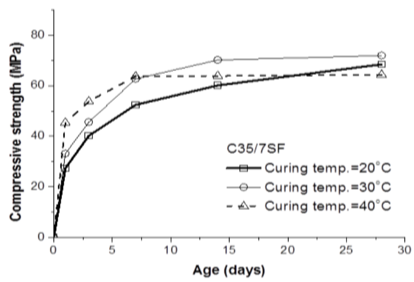
Additional ϕ100 × 200 mm cylindrical specimens were cast along with the shrinkage specimens of 100 × 100 × 400 mm to investigate the development of the mechanical properties of concrete like the compressive strength, elastic modulus, and splitting tensile strength of the concrete under different isothermal curing conditions (20, 30, and 40℃).

Table 3 Results of mechanical properties

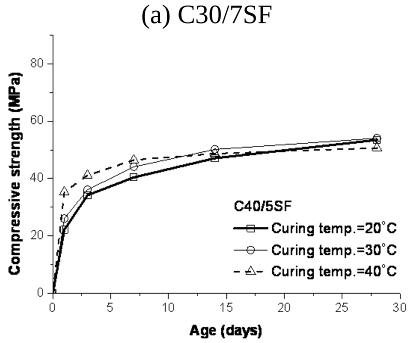
Mix ID	Age (days)	Compressive strength (MPa)			Splitting tensile strength (MPa)			Elastic modulus (GPa)		
		Curing temperature (℃)								
		20	30	40	20	30	40	20	30	40
C30/7SF	1	33.71	38.09	48.70	4.39	4.85	5.68	26.21	26.93	30.97
	3	45.12	53.28	62.55	5.94	6.09	7.04	32.48	33.45	36.69
	7	55.19	62.88	68.56	6.25	6.55	6.98	33.97	37.67	37.26
	14	63.72	73.10	70.57	6.57	6.95	6.99	35.89	39.10	36.95
	28	73.58	76.11	69.35	6.68	6.72	6.59	37.65	38.26	39.30
C35/7SF	1	27.36	33.18	45.41	3.56	4.05	5.01	24.75	27.92	30.34
	3	40.25	45.60	53.81	4.85	5.19	5.60	29.33	31.47	35.90
	7	52.43	62.74	63.73	5.36	5.92	5.87	32.28	34.78	35.62
	14	60.16	70.19	63.88	6.44	6.70	6.52	34.58	37.30	35.85
	28	68.47	71.94	64.36	6.54	6.47	6.27	35.47	36.98	37.63
C40/5SF	1	22.21	26.08	35.36	3.02	3.51	4.51	21.42	24.01	26.70
	3	34.21	36.12	41.20	4.12	4.61	4.98	24.78	27.81	30.02
	7	40.45	44.11	46.51	4.98	5.26	5.20	27.69	29.01	31.78
	14	47.13	50.19	48.72	5.34	5.46	5.32	28.38	30.76	32.56
	28	53.48	54.11	50.71	5.54	5.68	5.41	29.77	33.56	32.98
C40	1	19.99	21.80	29.40	2.76	2.98	3.48	20.77	22.33	24.34
	3	32.08	34.90	37.98	3.20	4.03	4.32	23.96	26.26	28.01
	7	37.74	38.35	42.46	4.06	4.43	4.56	25.47	27.01	28.33
	14	44.51	42.50	45.91	4.42	4.26	4.44	27.45	27.56	30.13
	28	48.45	47.76	48.46	4.72	4.54	4.46	28.87	30.34	30.33



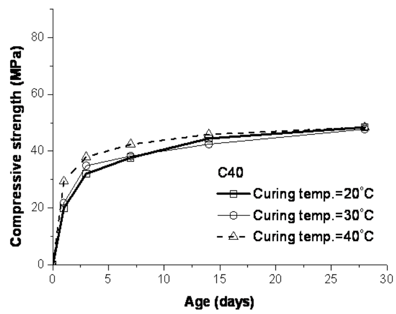
(a) C30/7SF



(b) C35/7SF

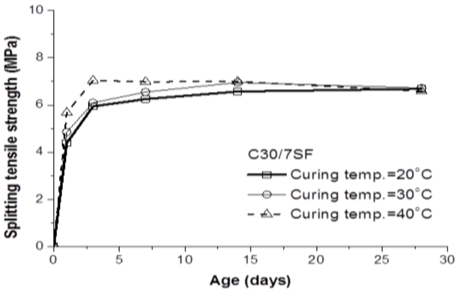


(c) C40/5SF

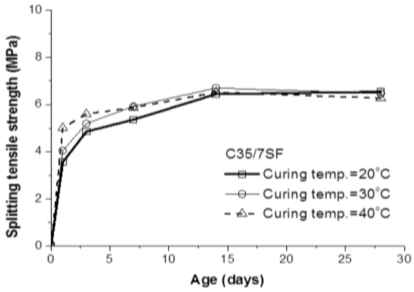


(d) C40

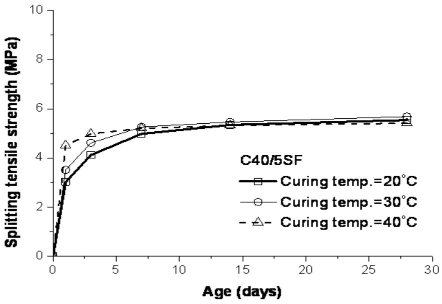
Fig. 1 Test results of compressive strength



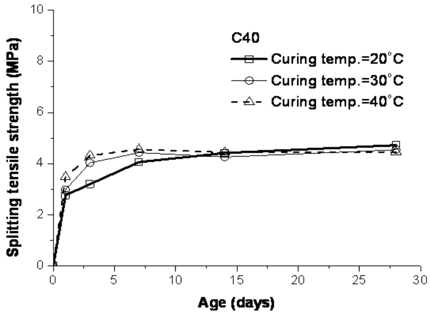
(a) C30/7SF



(b) C35/7SF

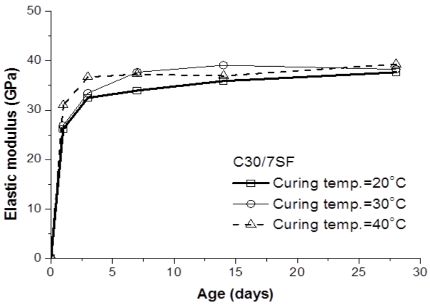


(c) C40/5SF

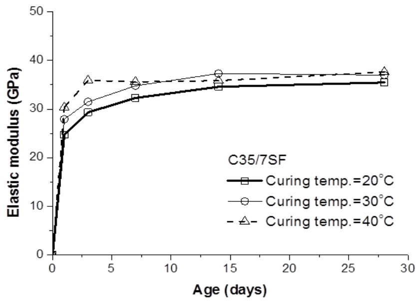


(d) C40

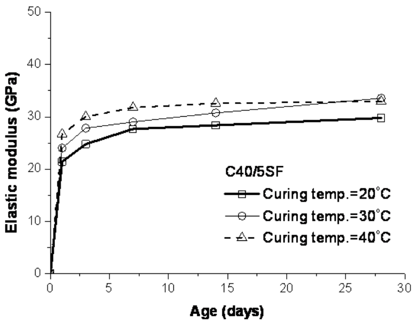
Fig. 2 Test results of splitting tensile strength



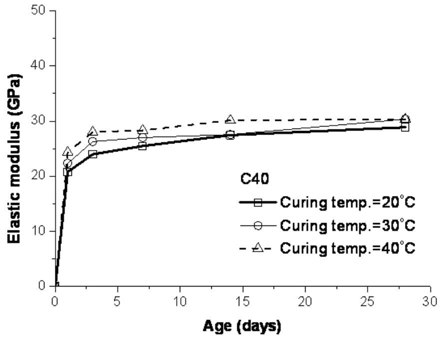
(a) C30/7SF



(b) C35/7SF

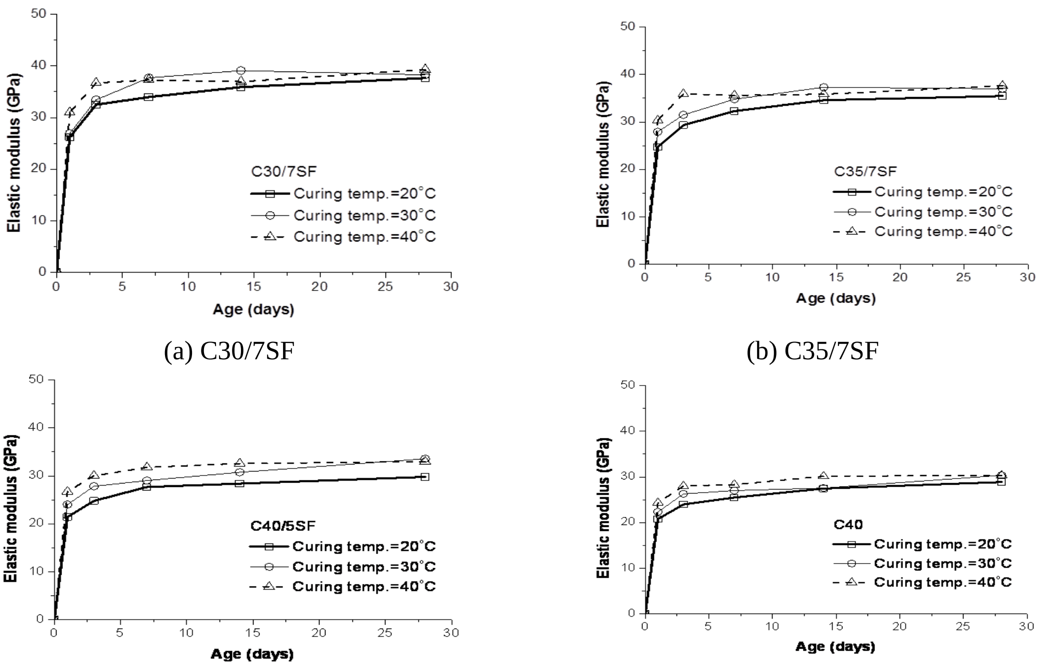


(c) C40/5SF



(d) C40

Fig. 3 Test results of elastic modulus



(a) C30/7SF (b) C35/7SF

(c) C40/5SF (d) C40

Fig. 4 Test results of autogenous shrinkage

3.2 Experimental results

Table 3 and Fig. 1 to Fig. 4 show the experimental results of each propertyfor four different concrete specimens. As shown in Fig. 1, the one- and three-day compressive strength levels increased with an increase in the curing temperature. However, this tendency was reversed with aging. The 28-day compressive strength of concrete cured at 40℃ is the lowest. These results suggest that concrete subjected to a high temperature at an early age attains a higher early-age compressive strength but a lower later-age compressive strength. Alexander and Taplin (1962) referred to this phenomenon as the "crossover effect". The same phenomenon also arises in the splitting tensile strength, elastic modulus, and autogenous shrinkage with increasing curing temperatures. However, the crossover effect of the splitting tensile strength and the elastic modulus is not as obvious as that of the compressive strength and autogenous shrinkage. This is due to the differences between the rates of increase for each property.

4. Application of prediction model

As mentioned previously, the increasing rates of the splitting tensile strength, elastic modulus, and autogenous shrinkage are dissimilar to that of the compressive strength. This dissimilarity must be considered in Eq. (1). The difference in the increasing rate can be estimated by modifying the constant *A* with determined properties. Following previous research (Kim *et al*. 2001), an *A* value in Eq. (1) of 1.0×10^7 is determined as the reference for the compressive strength. From the relationship between the relative compressive strength and each property, as shown in Fig. 5, the *A* value of each property can be determined. The values of the compressive strength, splitting tensile strength, elastic modulus, and autogenous shrinkage are 1.0×10^7, 3.0×10^7, 5.0×10^7, and 0.3×10^7, respectively. As shown in Fig. 5, the determined values of *A* can be used for the four different concretes because variations according to the mix proportion are small.

The age t_o in Eq. (1) is related to the starting point of the hydration reaction. Portland cement concrete remains in a plastic state for several hours after mixing, and the concrete during this period does not have a strength or elastic modulus. The compressive strength, splitting tensile strength, elastic modulus, and autogenous shrinkage will have the same value of t_o, as t_o is associated with the degree of cement hydration as well as the apparent activation energy.

Table 4 shows the regression results of the experimental data. Fig. 6 shows the variation of the apparent activation energy function with time for four different concrete specimenscured at temperature of 20℃. The results in Table 4 and Fig. 6 indicate that a high content of silica fume leads to a rapid decrease in the apparent activation energy, whichindicates adecrease in the hydration rate. The reason is that the silica fume acceleratesthehydration process at an early agebut decreases the hydration rate at later age (Neville 1995).

Based on the regression resultsshown in Table 4, the variation of each parameter with the curing temperature is presented and following general equationsis obtained.

$$\text{for C30/7SF} \quad E_o = 43{,}627 - 137T^c \quad \text{J/mole} \tag{2}$$

$$\alpha = 0.00029T^c \tag{3}$$

$$t_o = 0.498 - 0.014T^c \tag{4}$$

$$\text{for C35/7SF } E_o = 42{,}369 - 58\ T^c \text{ J/mole} \tag{5}$$

$$\alpha = 0.00025T^c \tag{6}$$

$$t_o = 0.440 - 0.011T^c \tag{7}$$

$$\text{for C40/5SF } E_o = 45{,}653 - 199\ T^c \text{ J/mole} \tag{8}$$

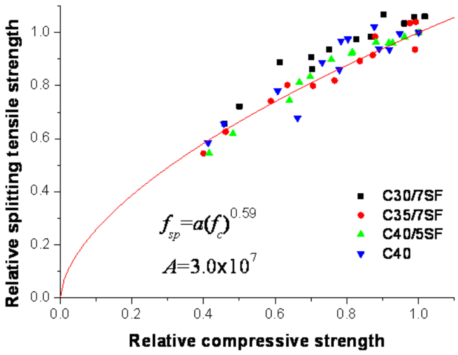
$$\alpha = 0.00022T^c \tag{9}$$

$$t_o = 0.848 - 0.022T^c \tag{10}$$

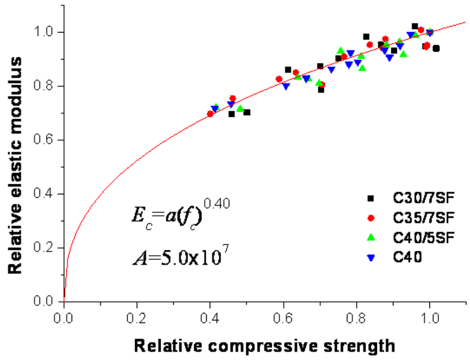
$$\text{for C40 } E_o = 45{,}208 - 164T^c \text{ J/mole} \tag{11}$$

$$\alpha = 0.00020T^c \tag{12}$$

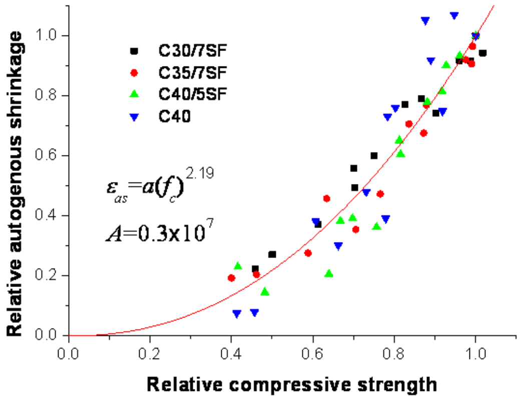
$$t_o = 0.905 - 0.021T^c \tag{13}$$



(a) Splitting tensile strength



(b) Elastic modulus



(c) Autogenous shrinkage

Fig. 5 Test results of autogenous shrinkage

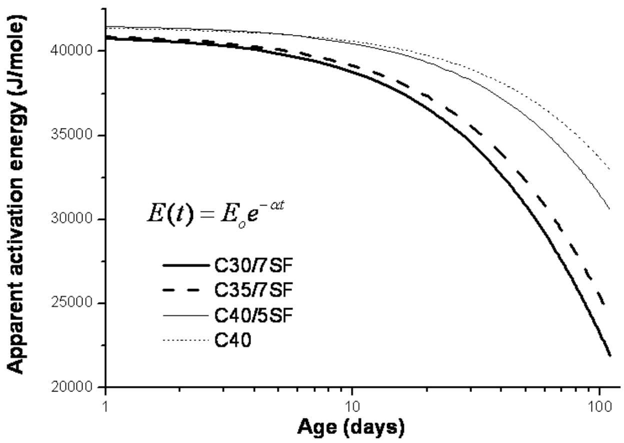
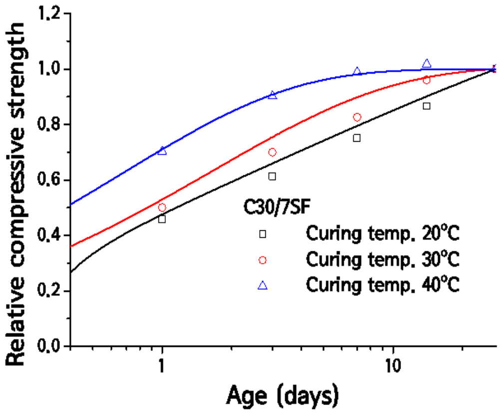
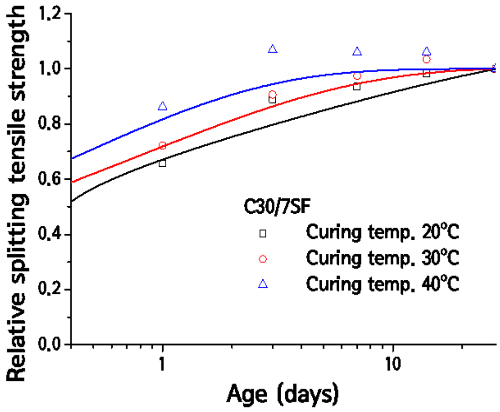


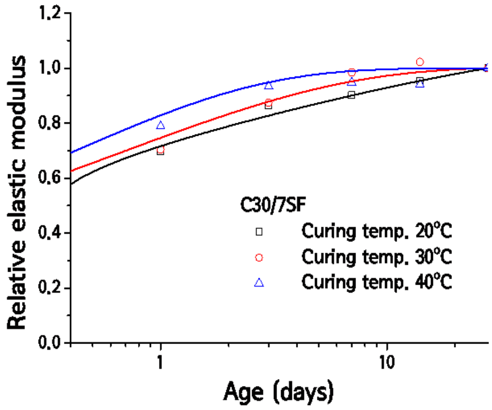
Fig. 6 Variation of apparent activation energy (curing temperature of 20℃)



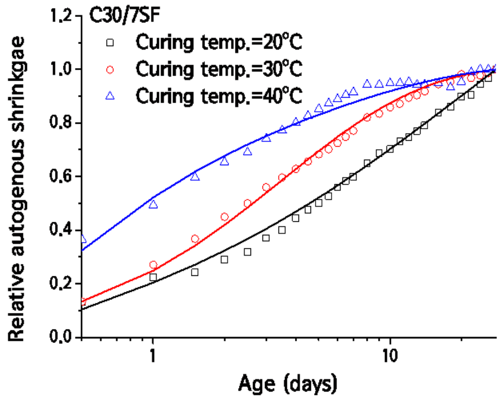
(a) Compressive strength



(b) Splitting tensile strength

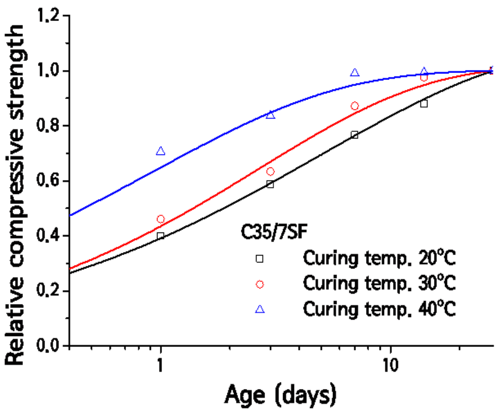


(c) Elastic modulus

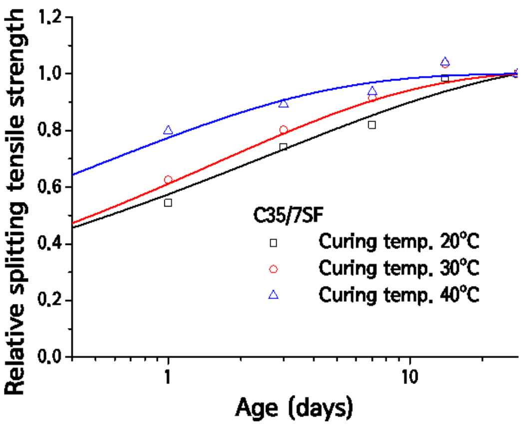


(d) Autogenous shrinkage

Fig. 7 Predicted values and experimental results (C30/7SF)

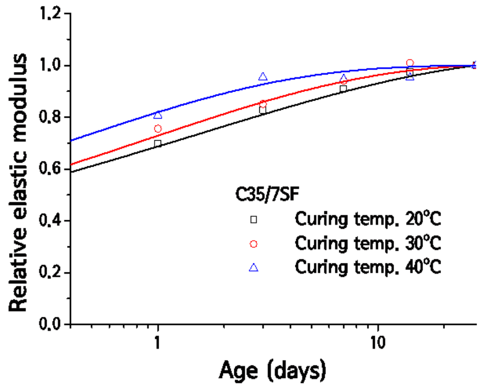


(a) Compressive strength

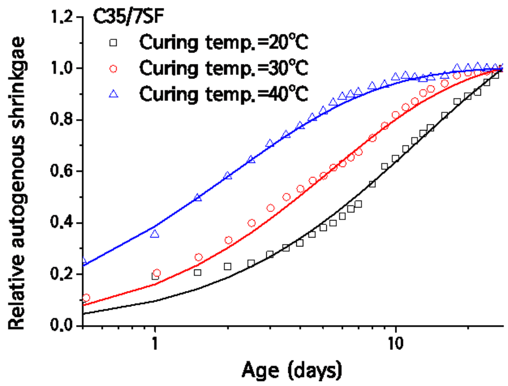


(b) Splitting tensile strength

Fig. 8 Predicted values and experimental results (C30/7SF)

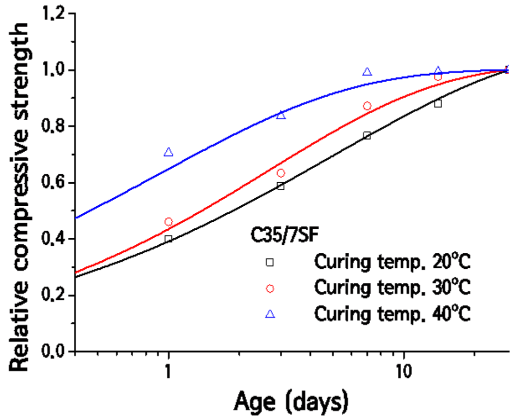


(c) Elastic modulus

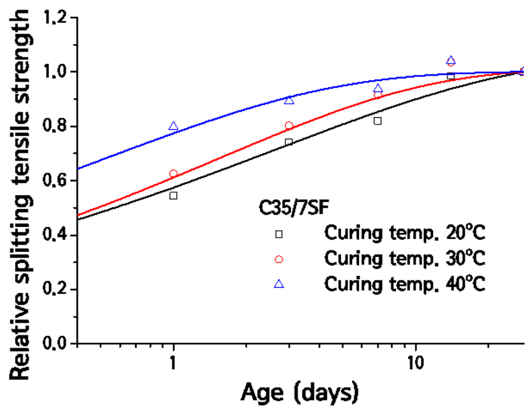


(d) Autogenous shrinkage

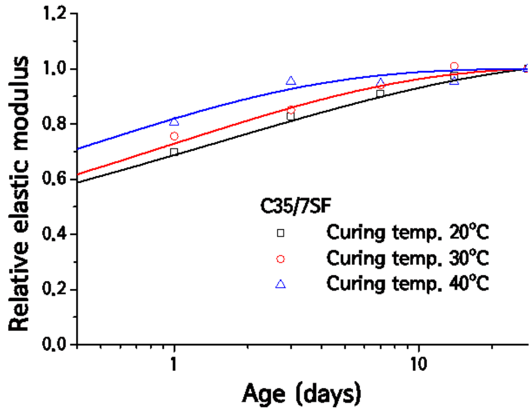
Fig. 8 Continued



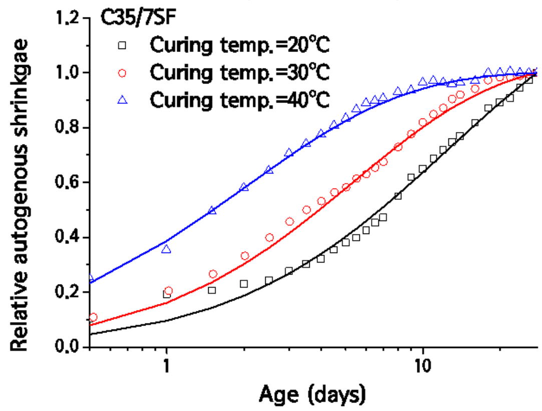
(a) Compressive strength



(b) Splitting tensile strength

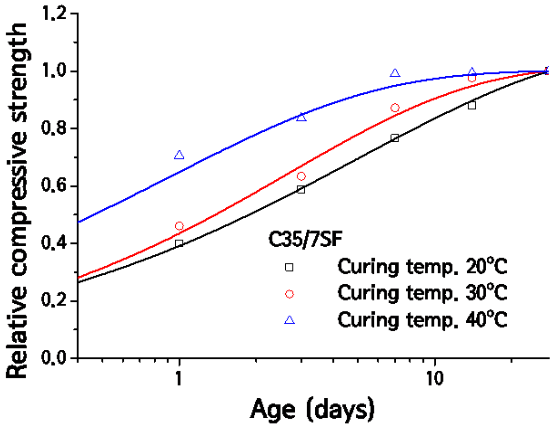


(c) Elastic modulus

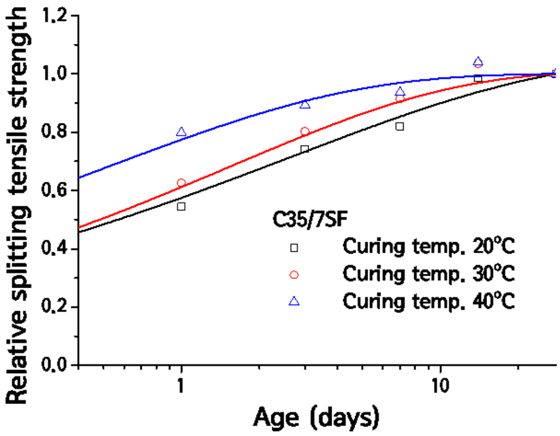


(d) Autogenous shrinkage

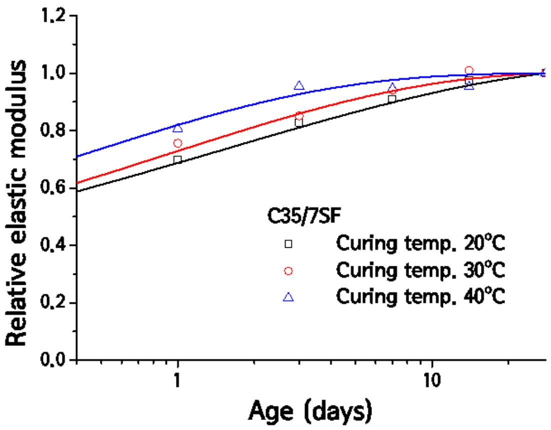
Fig. 9 Predicted values and experimental results (C30/7SF)



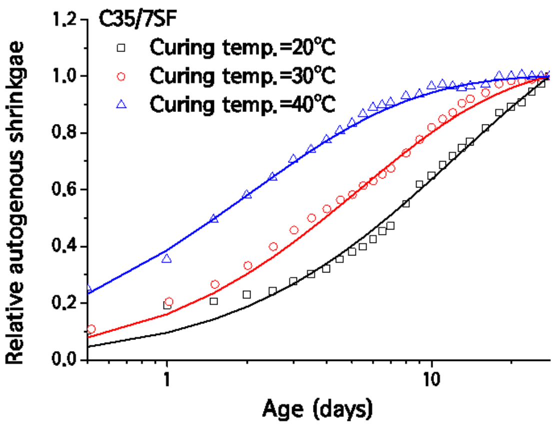
(a) Compressive strength



(b) Splitting tensile strength

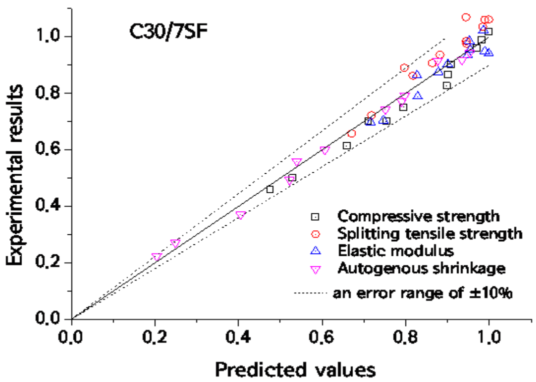


(c) Elastic modulus

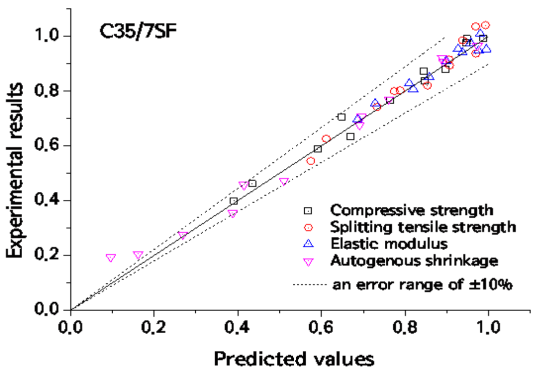


(d) Autogenous shrinkage

Fig. 10 Predicted values and experimental results (C30/7SF)

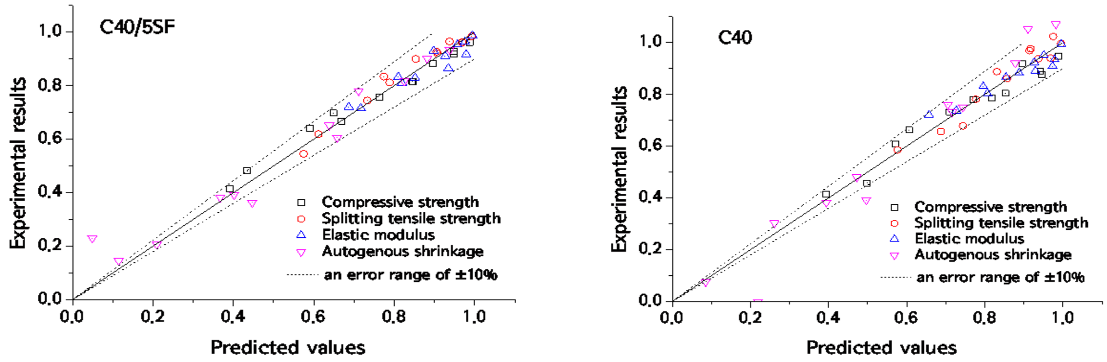


(a) C30/7SF



(b) C35/7SF

Fig. 11 Predicted values and experimental results (C30/7SF)



(c) C40/5SF (d) C40

Fig. 11 Continued

where, T^c is the curing temperature (°C).

Fig. 7 to Fig. 10 depict the predicted curves for the four different concrete specimens as well as the experimental results of the hydration-related properties, i.e., compressive strength, splitting tensile strength, elastic modulus, and autogenous shrinkage. In these figures, the scattered points denote the experimental results and the solid lines denote the predicted values. The differences between the calculated value and the experimental resultlikely arise because the regression results are based on a small number of test results excluding the results at a later-age. They also contain some degree of the experimental error in Figs. 7 (b) and (d). However, as shown in Fig. 11, the error range is less than ± 10 percent, which reflects that the prediction model properly estimates the hydration-related properties of concrete.

5. Relationships between splitting tensile strength and compressive strength or elastic modulus and compressive strength

In many existing codes, i.e., ACI 318 (American Concrete Institute 1999) and CEB-FIP model code 1990 (CEB-FIP 1993), a relationship between the splitting tensile strength and the compressive strength or the elastic modulus and the compressive strength are presented by following equations.

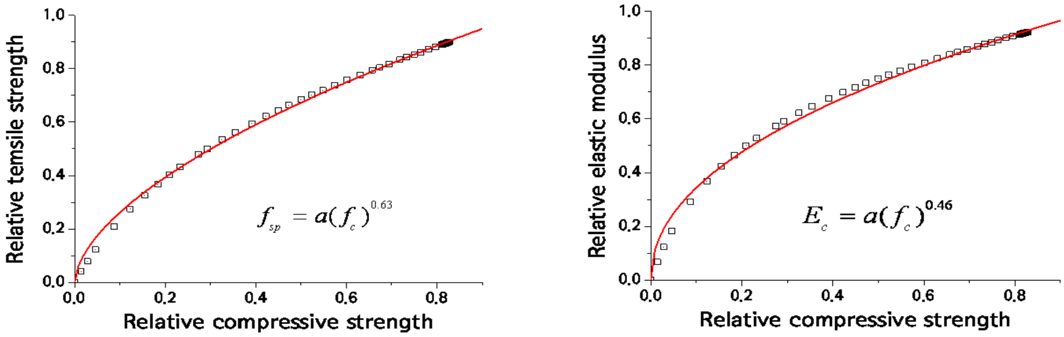
$$f_{sp} = \alpha \times (f_c)^b \tag{14}$$

$$E_c = \alpha \times (f_c) \tag{15}$$

where, f_{sp} is the splitting tensile strength, E_c is the elastic modulus, f_c is the compressive strength, *a* and *b* are empirical constants

In Eqs. (14) and (15), adissimilarity of increasing rate between the compressive strength and each property is considered by the value of *b*. ACI 318 suggests *b* values of 0.50 and 0.50 for the splitting tensile strength in Eq. (14) and the elastic modulus in Eq. (15), respectively. While, CEB-FIP model code 1990 suggests *b* values of 0.67 and 0.33 for the splitting tensile strength in Eq. (14) and the elastic modulus in Eq. (15), respectively.

The value of *b* is closely related to the value of *A* in Eq. (1). In the previous section, different



(a) Relationship between f_{sp} and f_c (b) Relationship between E_c and f_c

Fig. 12 Relationship between the compressive strength and each property

Table 5 Values of *A* corresponding to existing model codes

	Model equation	Values of *A* in Eq. (1)		
		for compressive strength	for splitting tensile strength	for elastic modulus
ACI 318	$f_{sp} = 0.56 f_{ck}^{0.50}$ $E_c = 4,700 f_{ck}^{0.50}$	1.0×10^7	3.7×10^7	3.7×10^7
CEB-FIP 1990	$f_{sp} = 0.30 f_{cu}^{0.67}$ $E_c = 8,480 f_{cu}^{0.33}$	1.0×10^7	2.1×10^7	6.5×10^7

values of *A* for each property were determined based on a regression analysis of the experimental results. The values of the compressive strength, splitting tensile strength, and elastic modulus were 1.0×10^7, 3.0×10^7, and 5.0×10^7, respectively. To obtain values of *b* corresponding to determined values of *A*, the relationship between the relative compressive strength and the relative values of each property were drawn in Figs. 12 (a) and (b). The determined values of *b* are 0.63 and 0.46 for the splitting tensile strength and the elastic modulus, respectively.

Also, the values of *A* corresponding to the existing model codes is determined. These values of A are tabulated in Table 5.

6. Conclusions

To investigate the validity of the prediction model, the model is applied to the hydration-related properties of the compressive strength, splitting tensile strength, elastic modulus,and the autogenous shrinkage. Based on results in this paper, the following conclusions were drawn.

1. Based on the assumption that the apparent activation energy is the characteristic property of concrete, a prediction model for compressive strength is applied to other hydration-related properties, i.e., the splitting tensile strength, elastic modulus, and the autogenous shrinkage. The predicted values by the model are compared with experimental results, and good agreement between the predicted values and the experimental results was observed within an error range of ±10 percent.

2. The proportional constant *A* is determined to predict different hydration-related propertiesofthe compressive strength, splitting tensile strength, elastic modulus, and the autogenous shrinkage. Determined values of *A* are 1.0×10^7, 3.0×10^7, 5.0×10^7, and 0.3×10^7 for compressive strength, splitting tensile strength, elastic modulus, and autogenous shrinkage, respectively.

3. An empirical constant *b* in existing model codes, which defines a dissimilarity of increasing rate between the compressive strength and each property, is closely related to the value of *A*in the prediction model. The values of *A* corresponding to existing model codes are determined.

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