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Relation between cement composition and compressive strength of pure pastes

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ABSTRACT

In Europe, cement paste compressive strength models are frequently described by a power law similar to that of Féret. The French LCPC has also adopted this mathematical approach in its recent concrete mixture proportioning model. However the coefficient *k* and exponent *b* of the adopted power law were calibrated with only one Portland cement clinker, starting from pure pastes with various concentrations. These parameters do not take into account the chemical properties of the clinker. The purpose of this work was to check if the clinker chemical nature had an influence on the mechanical performances of the pastes (at 28 days). Complementary tests with eight cements coming from six different cement plants were then carried out. The mathematical treatment of the results made it possible to connect coefficient *k* to the silica content of the clinkers and more particularly to their C_3S rates. It is linked to the strength of hydrated cement paste. Thus, the suggested approach significantly improves the accuracy of paste strength calculation. These results can be used to calculate concrete strength.

1. Introduction

Among the most used compressive strength calculation models – Abram's law, European methods like Féret's law and Bolomey formula – we have used the new concrete mixture proportioning model designed by the French Laboratoire des Ponts et Chaussées (LCPC) [1].

In this model, concrete strength is linked to that of cement paste taking into account parameters describing the effect of aggregates topology (paste–aggregate model) [2].

The 28-day compressive strength of pure cement pastes (fc_p) is calculated with a model similar to that of Féret [3]. This is a power law of exponent *b* whose C_0 variable is the cement concentration of fresh paste: the volume of cement in the volume of paste (Eq. (1)). Its main parameter is equal to the product of 28-day standard strength of cement σ'_{28} and coefficient *k* (Eq. (2)):

$$C_0 = \frac{v_c}{v_c + v_w + v_a} \tag{1}$$

v_c, v_w and v_a are the volumes of cement, water and air in fresh paste, respectively.

$$fc_p = \sigma'_{28} k C_0^b \tag{2}$$

To be able to predict paste strength starting from its composition in the concrete (quantities of cement, water and air), coefficient *k* and exponent *b* of the relation (Eq. (2)) were initially gauged by the LCPC [1] starting from tests on one pure cement paste. These tests consisted in measuring compressive strength at 28 days of a series of pastes made with only one cement CEM I 52.5 (95% of clinker, EN 197-1 norm) and various quantities of water (within the range $0.33 < C_0 < 0.58$). The fitting of the results provided values of 11.4 and 2.85 for *k* and *b*, with an average error of only 2.3 MPa [2].

In this model, parameters *k* and *b* are considered as valid for all cements whatever their chemical compositions may be. It means that the 28-day standard strength σ'_{28} is sufficient to differentiate mechanical behaviour in cement pastes. It would be interesting to consider other cement parameters such as their chemical compositions. Tsivilis and Parissakis showed that cement fineness mainly affects strength at early age (before 7 days) while chemical and mineralogical parameters influence strength at a later stage [4].

Previous studies have shown that the chemical properties of cement can influence many properties of the mixture such as its compressive strength. Brüggemann and Bentrup [5] have shown correlations between mineralogical clinkers parameters and cement strength. A relation linking compressive strength at 28 days to C_3S, C_2S, aluminates and ferrite contents has been developed by Knöfel [6]. Tsivilis and Parissakis [4] have presented three laws to determine compressive strength at three ages (2, 7 and 28 days) in relation with the clinker compounds and/or the fineness parameter. Jons and Osbaeck [7] have also given relations between cement composition and cement paste strength suggesting that clinker phases contribute to increasing strength as well as reducing porosity. Then the influence of micro structural porosity on cement paste has been shown in several models such as a law taking into

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account the porosity of cement paste either fresh or hardened to calculate compressive strength [8]. We note that the chemical differences between several clinkers may change the chemical equilibrium and thus the composition and structure of hydrates, which is contradictory to the single relation defined by the LCPC.

In this context, the purpose of this paper was to carry out complementary mechanical tests with several cements to check if the relation (Eq. (2)) can be improved by taking into account the clinker chemical composition. The results will then be used to find correlations between the parameters of the model and the cement chemical characteristics. Primarily, this study presents the material ingredients used to carry out the tests. Secondly, it presents the tests of reference [2], the tests carried out within the framework of this study as well as their material and instrumental environment. Thirdly, the obtained results are discussed. They made it possible to propose a more comprehensive approach of the compressive strength behaviour of pure cement pastes.

2. Material ingredients

The study was carried out with eight Portland cement clinkers (or type CEM I cements, according to the European standard EN 197-1). These cements were provided by six cement plants located in France, Luxembourg and Germany. Table 1 gives a letter to each cement from A to H as well as their commercial designations and their origins (numbers 1–6). Let us note that cement D comes from the same cement plant and thus should have the same characteristics as that used in the initial tests carried out by the LCPC [2].

The samples used in the tests came from recently manufactured cements. These samples were preserved in hermetic bags or pots until use (a few weeks after production). Their physical and chemical properties (specific density ρ_c, oxides contents) were given by the cement plant's quality control department. The specific densities vary from 3.13 to 3.18 tons per cubic metre. The compositions were also provided by the cement plants. The real contents of C_3S, C_2S, C_3A, and C_4AF in cement were obtained by X-ray diffraction investigations (XRD) according to the Rietveld method [9]. They generally differ from the theoretical values calculated with the Bogue equations for the clinker because of the presence of sulphate and possibly of calcium carbonate in cement and of the actual purity level of the clinker phases. The compressive strength (28-day standard strength σ'_{28}) of each cement was measured several times on standardized mortars according to European standards (EN 196-1). All values are given in Table 2.

Table 1
Reference and designation of cements.

Reference	Designation	Cement plant no.
A	CEM I 52.5 R	1
B	CEM I 52.5 R	2
C	CEM I 52.5 R	3
D	CEM I 52.5 N PM	4
E	CEM I 52.5 R	5
F	CEM I 52.5 N	5
G	CEM I 42.5 R	6
H	CEM I 42.5 R	2

CEM I: category; 52.5: cement strength (MPa); R: quick setting; N: normal setting; PM: sea setting.

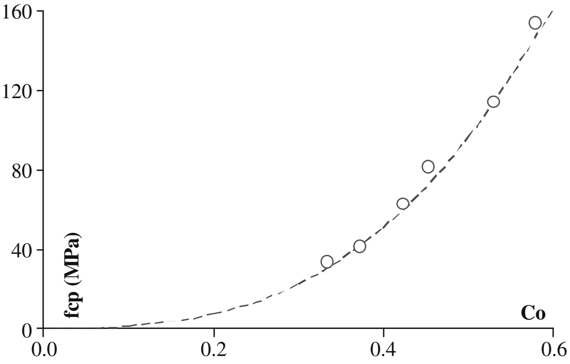

Fig. 1. Experimental values and fitting for the establishment of the initial law [2].

It is noted that major elements (SiO_2, Al_2O_3, Fe_2O_3 and CaO) are obviously constant from one cement to another. However, their compositions present significant variations. For example, the contents of C_3S and C_3A, respectively vary between 51% and 68% and between 2% and 14%.

One concrete superplasticizer – polycarboxylate water reducer – was used to cast the mixtures of low w/c ratio. It has a density of 1.05 and a solid content of 20%. The initial water content of this product was taken into account in calculations.

The different mixtures were made with distilled water to avoid possible differences caused by the water's chemical composition.

3. Experiments and results

3.1. The initial tests carried out by LCPC [2]

These initial tests were carried out by the French LCPC with cement whose origin and category are those of cement D. However, this cement had been manufactured twelve years before this study and its chemical composition could not be recovered. It is undoubtedly different from that of current cement D. Six pastes with different volumetric cement concentrations C_0 were mixed. They varied between 0.33 and 0.58. The pastes of low volumetric cement concentration (high w/c ratio) were mixed in two stages in order to avoid a bleeding phenomenon [10]. A diluted paste – of w/c ratio equal to 5 – was first mixed for 24 h. The obtained suspension con-

Table 2
Composition, hydraulic index (I), surface area (S.a.), 28-day standard strength of cement (σ'_{28}) of the used cements.

Ref	Oxide rate (%)								Composition (%)				I	S.a.	σ'_{28}
	SiO_2	Al_2O_3	Fe_2O_3	CaO	MgO	K_2O	Na_2O	SO_3	C_3S	C_2S	C_3A	C_4AF		cm^2/g	MPa
A	20.5	5.2	2.3	64.7	1.0	1.2	0.1	3.7	66.9	8.0	14.1	4.4	0.43	4510	62.7
B	21.0	6.0	2.5	63.5	–[b]	–[b]	0.44[a]	–[b]	67.5	7.0	6.0	10.0	0.46	4400	61.7
C	19.9	4.5	3.0	61.9	4.6	1.3	0.3	3.8	58.0	–[b]	8.0	10.0	0.41	5000	64.0
D	21.3	3.5	4.2	65.0	0.9	0.3	0.1	2.7	63.2	13.3	2.0	12.9	0.44	3550	60.4
E	19.8	5.1	3.0	63.5	1.7	0.9	0.2	3.3	54.5	19.2	8.4	9.8	0.43	–[b]	66.0
F	19.8	5.1	3.0	63.5	1.7	0.9	0.2	3.3	55.5	18.2	8.4	9.8	0.43	–[b]	64.2
G	20.0	5.5	3.1	63.0	3.0	1.4	–	3.6	51.0	22.0	9.0	10.0	0.43	4500	60.7
H	21.0	6.0	2.5	63.5	–[b]	–[b]	0.44[a]	–[b]	67.5	7.0	6.0	10.0	0.46	3350	55.1

[a] Alkaline components in the term of equivalent Na_2O.
[b] Values not given.

taining hydrated cement particles was then used like mixing water to make prismatic specimens (dimensions: 3.8 × 3.8 × 7.6 cm). The pastes of strong packing densities (low w/c ratio) were mixed with a moderate quantity of melamine type superplasticizer to facilitate casting. The paste specimens were extracted from their moulds after 2 days then rectified and ground smooth on a lapidary before being covered with an impervious membrane in order to avoid desiccation. Compressive strength values obtained at 28 days are reproduced on Fig. 1. They result from the average of the four tests. The results made it possible to obtain the initial parameters of the model (Eq. (3)) – i.e. $k = 11.4$ and $b = 2.85$ – with a small average error (2.3 MPa)

$$fc_p = \sigma'_{28} \times 11.4 \times C_0^{2.85} \tag{3}$$

3.2. Complementary tests: procedures and results

As for the initial study, the tests were carried out on pure cement pastes of various cement concentrations C_0. These tests are particularly difficult to carry out taking into account inherent difficulties of cement pastes: bleeding and segregation of fresh suspension; rise in temperature during the setting and hardening; drying shrinkage; regularity of the bearing surfaces for the mechanical tests; etc. To realize this study, original processes had to be tested and used such as the rotation of the paste during setting, its preservation in a confined environment and a great accuracy of rectification of the bearing surfaces before strength tests.

For each cement, eight series of six mixtures (12 for cement D) were prepared with cement concentrations C_0 ranging from 0.31 to

Table 3
Characteristics and compressive strength of the mixtures. Superplasticized mixes are identified with *. Values considered as erratic ones are noted in italic.

	Ref	ρ_e (t/m^3)	v_a (l/m^3)	C_0	fc_p (MPa)	s (MPa)
A	M1	1.674	4	0.318	30.5	0.8
	M2	1.747	1	0.351	36.0	2.3
	M3	1.822	5	0.388	46.7	4.3
	M4	*1.932*	*0*	*0.438*	*47.0*	*3.3*
	M5*	2.054	4	0.496	85.2	4.7
	M6*	2.103	5	0.520	95.1	3.9
B	*M1*	*1.679*	*6*	*0.314*	*15.2*	*2.2*
	M2	1.747	6	0.345	27.7	0.9
	M3	1.827	8	0.383	35.2	1.3
	M4	1.941	3	0.433	56.5	1.5
	M5*	2.078	0	0.494	103.5	1.6
	M6*	2.184	32	0.557	122.0	0.2
C	M1	1.676	6	0.316	19.1	1.9
	M2	1.746	5	0.347	30.8	0.9
	M3	1.831	3	0.386	33.0	3.4
	M4	1.936	2	0.435	53.4	4.1
	M5*	2.052	10	0.491	85.5	5.7
	*M6**	*2.123*	*41*	*0.539*	*73.1*	*7.9*
D	M1	1.678	7	0.314	12.7	1.6
	M2	1.745	7	0.345	29.8	0.3
	M7	1.790	7	0.366	40.1	1.0
	M3	1.825	9	0.383	42.4	2.1
	M8	1.880	8	0.408	49.6	5.0
	M4	1.936	5	0.432	51.5	4.6
	M9	2.016	0	0.466	65.0	7.5
	M5*	2.079	0	0.495	69.8	16.0
	M10*	2.171	0	0.537	117.1	7.0
	M6*	2.240	7	0.572	123.6	6.6
	M11*	2.304	32	0.579	126.9	5.0
	M12*	2.355	49	0.590	120.5	3.8
E	M1	1.675	7	0.315	17.8	1.5
	M2	1.733	12	0.345	22.4	1.6
	M3	1.829	4	0.386	35.5	3.4
	M4	1.935	3	0.434	43.6	3.9
	M5*	2.069	2	0.495	71.5	3.0
	M6*	2.168	21	0.550	91.6	0.9
F	M1	1.686	0	0.318	20.7	0.5
	M2	1.741	7	0.346	29.2	0.6
	M3	1.837	0	0.388	42.5	0.8
	M4	1.941	0	0.436	46.1	2.7
	M5*	2.072	0	0.496	82.8	2.6
	M6*	2.176	16	0.552	93.6	2.8
G	M1	1.681	4	0.316	18.6	0.5
	M2	1.750	3	0.347	24.4	1.0
	M3	1.837	1	0.386	37.4	4.7
	M4	*1.941*	*1*	*0.434*	*37.2*	*2.1*
	*M5**	*2.051*	*12*	*0.489*	*54.4*	*4.9*
	M6*	2.124	29	0.531	81.3	3.9
H	*M1*	*1.681*	*4*	*0.316*	*14.4*	*1.2*
	M2	1.745	6	0.346	26.5	0.6
	M3	1.825	8	0.384	36.1	2.2
	M4	1.941	1	0.434	53.5	5.2
	M5*	2.076	0	0.495	92.9	8.6
	M6*	2.205	21	0.564	129.2	10.9

0.59 (Table 3). It corresponds to w/c ratios ranging from 0.70 to 0.22 (Eq. (7)). To avoid a possible mechanical effect of the hydrated cement particles caused by the use of highly diluted paste as mixing water (initial tests carried out by the LCPC, 3.1), pure pastes were mixed with distilled water. Paste mixing was carried out with a standardized mortar mixer according to EN standard 196-3. Each 1-litre mixture was used to fill two impervious cylindrical moulds especially built for these tests. They are very regular altuglass™ test tubes – 18 cm long with 5 cm large interior diameters – provided at each end with a threading intended to fix PVC seal plugs (Fig. 2). One of the two plugs was equipped with a sealable vent. After casting, each mixture was left to set and harden and was preserved 28 days in these tubes until testing.

During casting the moulds were vibrated with a mobile plate to eliminate as much entrapped air as possible. Filled moulds were sealed with round PVC plugs with vents leaving almost no air inside. Sealed test tubes were weighed in order to know experimental fresh densities ρ_e. They are given in Table 3 (in tons/m^3). By comparison with the theoretical fresh densities ρ_t deduced from the compositions, it is possible to estimate the entrapped volume of air in each mixture expressed in unit volume according to the following relation:

$$v_a = 1000 \times (1 - \rho_e/\rho_{t.}) \tag{4}$$

These volumes of air are also given in Table 3 in litres per cubic metre. They made it possible to calculate the real cement concentration C_0 of each mixture (Eq. (5)).

$$C_0 = \frac{v_{\text{cinit}}(1 - v_a)}{v_{\text{cinit}}(1 - v_a) + v_{\text{winit}}(1 - v_a) + v_a};$$
$$C_0 = \frac{v_{\text{cinit}}}{v_{\text{cinit}} + v_{\text{winit}} + v_a/(1 - v_a)} \tag{5}$$

Therefore, the initial volumetric proportions of cement (v_{cinit}) and water (v_{winit}) in unit volume were adjusted by taking into account the volume of mixture actually produced

$$v_c = v_{\text{cinit}} \cdot (1 - v_a) \quad \text{and} \quad v_w = v_{\text{winit}} \cdot (1 - v_a) \tag{6}$$

The mixtures with high cement concentrations (or low w/c ratio) were cast in the presence of superplasticizer proportioned between 1% and 1.5% of the cement mass. This proportioning was voluntarily reduced to mitigate a potential disturbing effect such as a modification of the usual chemical reactions.

The mixtures of low cement concentrations (or high w/c ratio) naturally undergo segregation if they are maintained at rest. To avoid this phenomenon, the altuglass™ test tubes were placed in a particular setting device in slow and offset rotation (seven revolutions per minute) for the first 24 h. The longitudinal axes of the test tubes turned in a vertical plane around a horizontal axis located at ten centimetres from the centre of the mould (Fig. 2).

Fig. 2. Device intended to prevent the fresh cement paste segregation by slow rotation.

The test tubes were placed on the machine as soon as filling was finished. In respect to homogeneity all the mixtures underwent this treatment even the firmest. From the 24th hour to the release from the test tubes at 28 days, the sealed moulds were kept at a temperature of 20 ± 1 °C. A control of their masses over that period guaranteed that the pastes were not air dried.

The day of the tests, after removal from the tubes, the ends of the paste specimens were cut off from approximately 1 cm and then the specimens were sawn in half. The dimensions of the obtained cylindrical half-specimens were 5 cm wide and about 8 cm long. The bearing surfaces were rectified with a precision machine and carefully ground smooth. Flatness and parallelism of the supports were checked on a plate surface

For the compressive test, each half-specimen was subjected to a 0.5 MPa/s compressive rate until rupture (EN standard 12390). The results are given in Table 3. Each value is the average of the four measurements obtained on each mixture. The standard deviations of the results *s* are also given in Table 3.

3.3. Discussion

Fig. 3 presents the evolution of the estimated entrapped air volume according to cement concentration C_0. This volume remains low until a concentration of 0.50 (fluid mixtures). It becomes more important over that limit. The entrapped air volume goes from a few litres per m^3 (less than 10 l or 1%) up to 50 l per m^3. These tests show the difficulties in eliminating air in paste with high packing density and high plastic viscosity.

Fig. 4 presents, for each cement, the experimental strength compressive values at 28 days according to C_0. The dotted curves describe the theoretical evolution of strength according to the initial model (Eq. (2)) using the 28-day standard strength of each cement. It is noted that experimental fitting does not always satisfy the initial model. It is close for cements like B and H but for the others the measured performances deviate from the forecasts. For example, for cement E, the variation is about 10 MPa for low cement concentration and it exceeds 45 MPa for high cement concentration. In relative value, the theoretical strength of this cement paste is overestimated by almost 35%. For cement D, the performances are a little lower than the ones obtained by the LCPC although the cement used belongs to the same category (but not to the same production). Cements resulting from the same clinker (cement plants 2 and 5) logically present rather similar curves in spite of setting kinetics (R – quick– for E, N – normal – for F) and cement strength differences (52.5 for B, 42.5 for H).

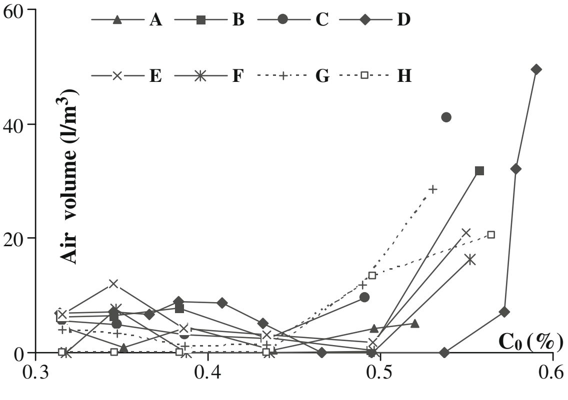

Fig. 3. Entrapped air volume in the different cement pastes.

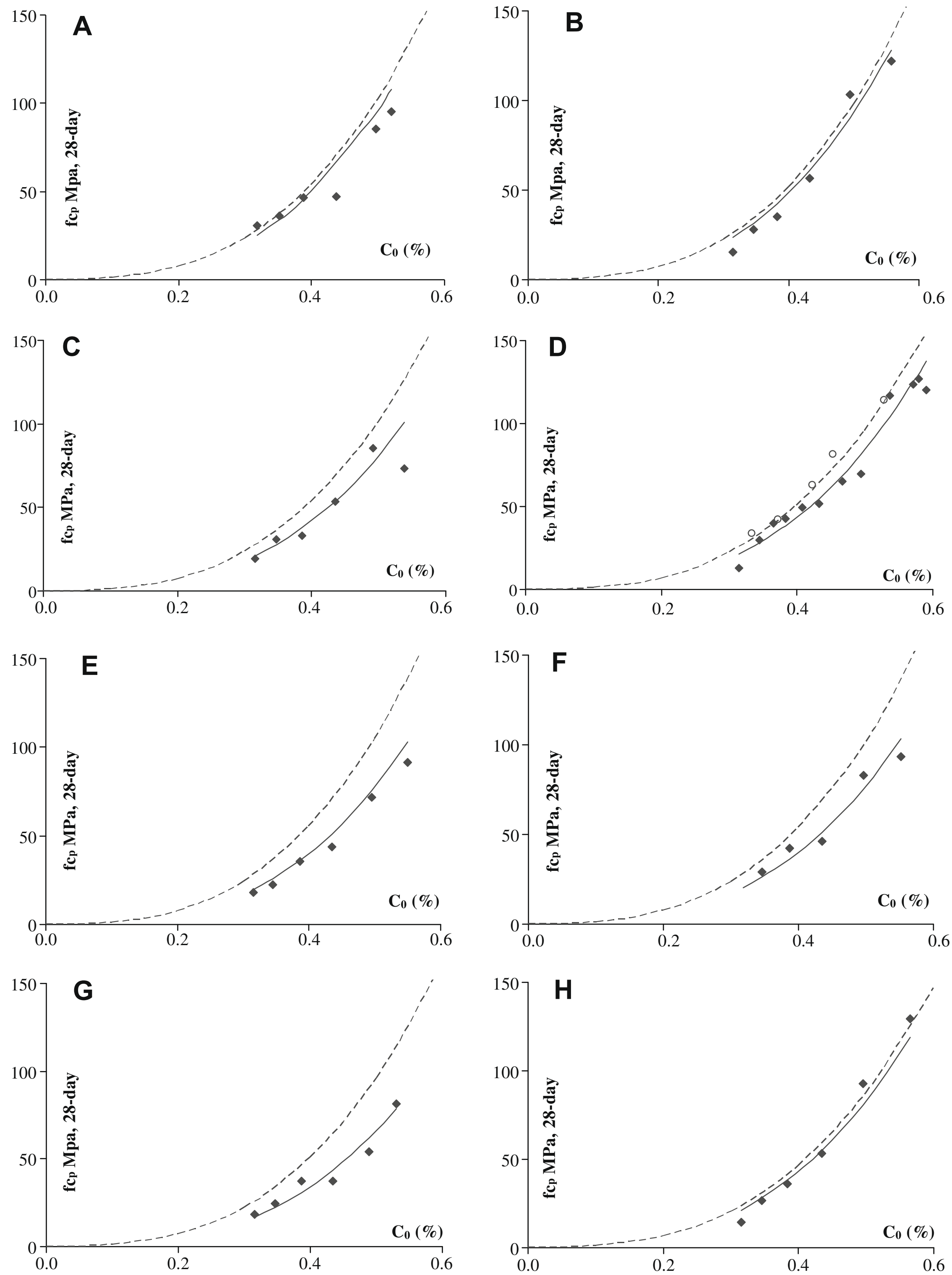

Fig. 4. Obtained experimental points and model's curves for the different cements. The initial model (Eq. (2)) is in dotted line, the new suggested model (Eq. (10)) is in fat For cement D, initial fitting points [2] are represented with white rounds.

Table 4
Fitting of the results gathered by cement strength.

Optimisation on	k and b			k with $b = 2.95$		b with $k = 10.5$	
	k	b	s (MPa)	k	s (MPa)	b	s (MPa)
CEM I 42.5	13.28	3.20	10.70	11.21	10.94	2.87	11.14
CEM I 52.5	9.47	2.86	8.79	10.07	8.84	3.00	8.91

Size effect [11,12] is a first hypothesis to explain the differences between our experimental test campaign and the initial one on cement D, which resulted in the theoretical model (see Section 3.1). Despite the difficult task of determining the actual impact of this phenomenon, we noticed that the bearing areas and volumes of the specimens are very similar in both experimental approaches. Only their forms differ. They were prismatic (3.8 × 3.8 × 7.6 cm) in the initial tests and cylindrical (5 cm wide and 8 cm long) in ours. Furthermore, in our experimental test campaign differences in compressive strength have been noticed between the different cements despite constant experimental conditions. Therefore, size and shape effects cannot explain the strength differences between these different cements.

Finally, for all cements, compressive strength measured on pure paste with cement concentration close to 0.40 are always lower than standard strength σ'_{28} measured on standardized mortar (comparison in Tables 2 and 3). The concentration of 0.40 is the one roughly corresponding to a w/c mass ratio of 0.50 (Eq. (7)). That is to say the cement concentration of the standardized mortar used to measure the 28-day standard strength cement. By neglecting entrapped air – small quantities are often observed – (Fig. 3) the relations between w/c and C_0 are as follows:

$$C_0 = \frac{1}{1 + \rho_c w/c} \quad \text{and} \quad w/c = \frac{1 - C_0}{\rho_c \cdot C_0} \tag{7}$$

Strength differences between pastes and mortars are explained by the aggregate topological effect on strength (maximum paste thickness, ceiling effect and bond effect of the grains, etc. [2]). However, these differences vary from one cement to another. This is an additional argument to justify that cement 28-day standard strength σ'_{28} is probably not a sufficient criterion to build a general model to forecast cement paste strength.

4. Influence of chemical composition

4.1. Adjustment of the model parameters

The model parameters (Eq. (2)) (coefficient *k*, exponent *b*) were optimized using the minimum standard deviation *s* on the ordinates (according to the approach of least squares). Primarily, these calculations were conducted on all disconcerted points including those of initial measurements [2] (except some values considered as erratic and announced in italics in Table 3). The aim was to find some satisfying constant averages. The found values are $k = 10.5$ and $b = 2.95$. These values are rather close to those of the initial parameters given in [2] but the associated standard deviation ($s = 11.7$ MPa) is too high to consider this solution as really satisfactory. Secondly, fitting curves were calculated by classifying cements according to two cement strengths (42.5 and 52.5). Thirdly, fitting curves were independently drawn for each cement. Table 4 and Table 5 give the results. Three simulations were conducted for each case. For the first one, both parameters k and b could simultaneously vary. For the two others, exponent b previously found ($b = 2.95$) was kept constant whereas coefficient k was optimized, then the converse was done ($k = 10.5$). The standard deviations *s* between experimental and theoretical compressive strengths were calculated for each adjustment. They were selected to choose the most relevant fitting curves.

On the one hand, sorting out cement strengths (either 42.5 or 52.5 in Table 4) does not make this model more accurate than the initial one (higher standard deviations and divergent *k* and *b* parameters). On the other hand, when fitting curves are calculated for each cement (Table 5), standard deviations are reduced of more than half whatever the simulation type used. Moreover, cements of similar chemical nature have relatively similar parameters (B and H of cement plant 2; E and F of cement plant 5). The improvement of paste strength calculation model thus probably works by taking into account the physicochemical characteristics of each cement used.

Among the three calculation modes used in Table 5, the one where k and b vary simultaneously offers the best accuracy (average standard deviation of 3.80 MPa). But this solution comes down to having to adjust two parameters for each cement. To simplify, exponent b has been kept constant ($b = 2.95$) while coefficient *k* has been linked to the chemical properties of cements. Furthermore, according to the calculations presented in Table 5, exponent b gives a better statistical stability ($s'/m = 0.07$) and coefficient *k* a better accuracy (average standard deviation of 4.85 MPa, that is to say a value close to that found when *k* and *b* are simultaneously optimized).

Table 5
Fitting of the results for each cement used

Optimisation on	*k* and *b*			*k* with $b = 2.95$		*b* with $k = 10.5$	
	(1)	(2)	(3)	(4)	(5)	(6)	(7)
	k	*b*	*s* (MPa)	*k*	*s* (MPa)	*b*	*s* (MPa)
A	7.13	2.40	0.74	10.62	4.84	2.92	4.64
B	12.52	3.07	7.64	11.56	7.74	2.82	8.09
C	14.87	3.41	3.06	10.23	4.15	2.99	4.00
D	10.52	2.90	6.73	10.87	6.75	2.90	6.73
E	7.99	2.91	2.17	8.24	2.19	3.29	3.37
F	6.75	2.52	4.97	9.11	5.96	3.14	6.86
G	7.18	2.65	1.53	8.92	2.58	3.17	3.86
H	15.23	3.24	3.52	12.56	4.60	2.71	6.66
Average m	10.27	2.89	3.80	10.26	4.85	2.99	5.53
Standard deviation s'	3.5	0.4	–	1.4	–	0.2	–
s'/m	0.34	0.12	–	0.14	–	0.07	–

Table 6
Correlation coefficients *R* enters the coefficient *k* ($b = 2.95$) and chemical compounds of cements and specific area (s.a.).

Compound	SiO_2	Al_2O_3	Fe_2O_3	CaO	I	SiO_2/CaO	C_3S	C_2S	C_3A	C_4AF	s.a.
R	0.845	0.221	−0.237	0.198	0.713	0.901	0.896	−0.904	−0.326	0.016	−0.632

4.2. Relation with the cement composition

Primarily, several linear adjustments of coefficient *k* (column 4 of Table 5) and of the various parameters of cement chemical composition (Table 2) were tested. Cement chemical composition has been defined using oxide masses (SiO_2, Al_2O_3, Fe_2O_3, CaO) as well as Rietveld composition and the hydraulic index I ($I = (SiO_2 + Al_2O_3 + Fe_2O_3)/(CaO+MgO)$or in SiO_2/CaO ratio). The specific areas (S.a.) of the cements have also been adjusted in the tests. The obtained correlation coefficients R are given in Table 6. Let us recall that they correspond to the co variances of *k* and *x* divided by the product of the standard deviations of *k* and *x* (x being the series of values correlated to the values of *k*):

$$R = \frac{cov(k,x)}{s_k \times s_x} \quad \text{or} \quad R = \frac{\overline{k \times x} - \bar{k} \times \bar{x}}{s_k \times s_x} \tag{8}$$

Fig. 5 shows fitting curves for C_2S, which present the best correlation ($R = -0.904$). This coefficient R is almost as good for ratio SiO_2/CaO ($R = 0.901$) and for C_3S ($R = 0.896$). It is still good for SiO_2 ($R = 0.845$). On the contrary, it is not good for the hydraulic index I ($R = 0.713$) or the specific area ($R = -0.632$) and even worse for all the other chemical elements. From a physical point of view, the link between the strength of pure paste and its content in siliceous elements (C_3S, C_2S, SiO_2) can be explained by the fact that hydrates (HSC – tobermorite) come from these phases, which are mainly responsible for the material's compressive strength [13] [14].

According to these results, three (linear) relations can be defined to determine parameter *k* with good accuracy, starting from Rietveld analysis or cement chemical analysis:

$$k = -0.22 \cdot [C_2S] + 13.28 \tag{9}$$

$$k = 160 \cdot [SiO_2/CaO] - 41.2 \tag{10}$$

$$k = 0.2 \cdot [C_3S] - 1.65 \tag{11}$$

It will be noticed however that parameter "C_3S" represents the most abundant phase in the clinker. Its variation range is also the largest (between 50% and 70% for the cements used in this study). Therefore, this parameter has been chosen in the model to describe the strength of a cement paste (at 28 days) as follows (Eq. (12)), by the combination of Eqs, (2) and (11):

$$fc_p = \sigma'_{28}(0.2.[C_3S] - 1.65)\left(\frac{v_c}{v_c + v_w + v_a}\right)^{2.95} \tag{12}$$

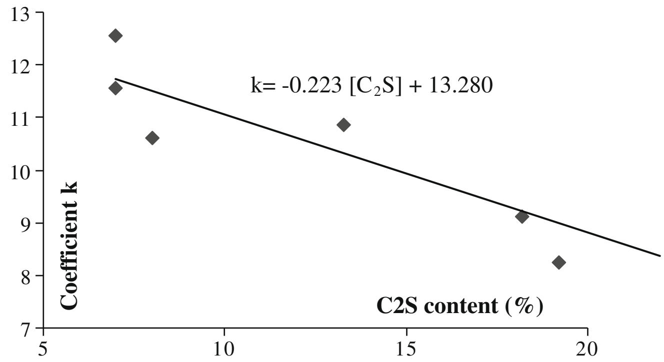

Fig. 5. Relation between parameters *k* ($b = 2.95$) and the cement C_2S content.

4.3. Comparison between the initial model and the new one

The new model (Eq. (12)) was compared with the initial one (Eq. (3)), [2] by plotting the new theoretical curves on Fig. 4 (full features) and by calculating the standard deviations with the experimental points (Table 7).

Most of the time, the new model predicts a much more relevant experimental compressive strength. Compared to the initial model, the error is overall reduced of more than half (*s* goes from 15.75 to 6.87) and it is often similar to that of the individual adjustments. This new model allows a better estimation of compressive strength by taking into account the chemical composition of cement.

This is an improvement of the compressive strength prediction model of cement pastes and thus of that of concretes defined by the LCPC in [2]. Several tests are currently carried out to evaluate the relevance of this new approach regarding high performance concrete strength calculations.

5. Conclusion

Compressive strength of a pure cement paste at 28 days is mainly controlled by the 28-day standard strength of this cement. But this study shows the importance of its chemical composition, in particular the amount of C_3S, which reflects the quantity of silicon present in the clinker. Let us recall that the content of C_3S taken into account in this paper was determined by treatment of analyses XRD according to Rietveld method. Indeed, the many tests carried out and the equations that have been defined (Eqs. (9) – (12)) showed that for equivalent 28-day standard strength, cements rich in C_3S produced the strongest pastes. It confirms the fact that hydrates resulting from this cement constituent are mainly responsible for the strength of the product. In this hypothesis, coefficient *k* and sometimes *b* depend on the chemical composition of the clinker (high values of the correlation coefficients). Thus, cement probably has the same value for *k* (at a defined time: 28 days for example) whatever its standard strength, which depends on its granulometry and its specific area. In other words, two cements from the same clinker production have the same value of *k* despite their different standardized cement strength (depending on grain fineness).

This taking into account of the cement chemistry in a model similar to that of Féret (power-law) was done by correlating the content of C_3S with the parameter of the law, its constant exponent b being kept. Other correlations are also possible using C_2S or silicon content.

The use of this comprehensive model is not particularly harder because the necessary data are generally available on the cement chart. It could have a practical application to calculate the strength of high performance concrete (paste with high cement concentration). Then a significant variation of *k* leads to a significant change of paste compressive strength and consequently of concrete strength.

In a future paper, these results will be checked on concretes of identical composition composed of various cements. The evolution of these parameters over time may also be studied.

Table 7
Standard deviations *s* between experimental points and strength theoretical values calculated according to the initial model and the model suggested.

Model	A	B	C	D	E	F	G	H	Global
Initial	10.53	9.10	12.57	14.95	26.29	20.70	17.84	5.78	15.75
Suggested	7.37	7.76	4.70	8.14	5.98	6.06	3.76	7.30	6.87

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