ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

The Chemical Composition Modeling of Cement CPJ_{55}

N. Mtarfi[1*], Z. Rais[1], M. Taleb[1], R. Elmrabet[2], S. Naamane[1], K.M. Kada[3], M. Assouag[4], and A. Zarrouk[5]

[1] Laboratory of Engineering, Electrochemistry, Modeling and Environment (LIEME), University Sidi Mohamed Ben Abdellah, Fes, Morocco.
[2] Laboratoire de la Chimie de l'Etat Solide, Faculté des Sciences, Université Ibn Tofail, Kénitra, Morocco.
[3]Quality Control Department, Cimenterie ASMENT TEMARA, Temara, Marocco.
[4] Equipe Matériaux Avancés et Applications ENSAM, Université Moulay Ismail, B.P. 15290 Al Mansour, Meknès, Morocco.
[5] LCAE-URAC 18, Faculty of Science, First Mohammed University, PO Box 717, 60 000 Oujda, Morocco.

ABSTRACT

The growing demand of cement CPJ_{55} requires better quality product. In this paper, it is aimed to propose prediction approaches for the 2, 7 and 28 days compressive strength of Portland composite cement (PCC) by using soft computing techniques. Plant data were collected for 8 months for the chemical and physical properties of the cement that were used in model construction and testing. The training and testing data were separated from the complete original data set by the use of Multilinear regression (MLR) model based on the training data of the cement strength was created. Testing of the model was also done within low average error levels (2.14; 2.83 and 1.89%), respectively. The three models were subjected to sensitivity analysis to predict the response of the system to different values of the factors affecting the strength. The utility of the model is in the potential ability to control processing parameters to yield the desired strength levels and in providing information regarding the most favorable experimental conditions to obtain maximum compressive strength. The results obtained from the computational tests have shown that MLR is a promising technique for the prediction of cement strength.

Keywords: Cement CPJ_{55}, compressive strength, Portland composite cement, Multilinear regression, prediction

Corresponding author

INTRODUCTION

Compressive strength of Portland cement mortar is the major property that defines its quality and depends on several factors that need to be controlled during manufacture. These factors range from the C_3S content to the fineness of the milled product and have varying degrees of effect on strength [1]. An analytical model to describe the effects of each of these factors on strength can be very complex. Multilinear regression (MLR) [2] can be used for this purpose as a tool for prediction modelling of strength. Its use in other areas and has proved its feasibility but the use of the MLR for predicting the mortar strength of Portland cement compound has not been reported because the number of the input variables is very important to be studied.

However, the number of published papers on the subject is very small. Akkurt and al. [3] used NNs for the cement compressive strength (CCS) prediction. They also analyzed effects of various parameters on the 28-day strength. Fa-Liang [4] applied fuzzy logic to CCS prediction successfully. Other studies made use of regression analysis to predict the compressive strength (CS) of Portland cement CPA [3,5-10] applied regression methods for CCS prediction. Interestingly, the number of papers that make use of the regression analysis is also very small. There is no published work in the literature that makes use of Multilinear regression (MLR) approaches on the prediction of CCS. This paper makes such an attempt by using MLR [11,12] for the prediction of the compressive strength (CS) of the Portland cement compound -type CPJ_{55} from the percentages of the individual constituents, the chemical and mineralogical composition of the clinker.

The data were collected during 8 months of plant operation« ASMENT TEMARA-Morocco». Because the plant operational parameters occasionally vary, the data had some variations that must be taken care of before modelling. In other words, the average strength of the shipped product varied as a function of time. Therefore, we used the data for the first 6 months to establish the model and testing the quality of the model was tested with the data of the remaining 2 months. These data were used to create an adequate mathematical model to reach our goal.

MATERIALS AND METHODS

Materials

The 28 days compressive strength of Portland compound cement CPJ_{55} is equal to 55 MPa. These cements are prepared in cement plant "Asment Temara " and the compressive strength are calculated according to the Moroccan standard NM.10.01.005 [13] and the European standard EN 196-1 [14]. The initials components of those cements are: clinker, gypsum, limestone and fly ash.

Method

The estimation of compressive strengths of cement CPJ_{55}, according to three different ages was performed by stepwise backwards regression method (RML) [2]. The constructions of the linear model of principles are based on the least squares method to estimate the mathematical equation parameters established by MLR [15]. Indeed, this model requires the definition of two types of variables, endogenous and exogenous. The endogenous variables represent the input of the model and exogenous variables, the output of the model.

The rationale for the contribution of each variable in the model is performed by the Student test, Fisher, Durbin-Watson test and analyzing the Henry curve, after determining the significance level. For this, it was necessary to provide a training sample for model development and other for the test validation. The validation test of the predicted model is used to test if the effect of exogenous factors is significant or not, in addition to the study of the coefficients of multiple determination R^2 which one should get close to 1 (100 %). The experimental validation of the linear model is performed by evaluating the difference between the observed and predicted values of the dependent variable.

For a perfect model, this difference should be less than the standard error of the established model.

Data Collection

The data of the chemical and mineralogical composition of clinkers and compressive strengths of cements corresponding to CPJ_{55}, were collected from the company Asment Temara during an 8 months of plant operation (from January to August 2014). We defined 17 input variables of the mathematical model and 3 output variables which are the compressive strengths of 2, 7 and 28 days for the two types of cement (Table1).
The data of the first 7 months have been exploited to establish the model, and those of the 8th month are used to test the model validation.

RESULTS AND DISCUSSION

Determining variables

The studied cements CPJ_{55} consist of four materials: clinker, limestone, fly ash and gypsum. Each one of this material has his own physicochemical characteristics.

The chemical composition of this material is evaluated by measuring the magnesium oxide MgO, silica SiO_2, alumina Al_2O_3, iron Fe_2O_3, sulfur SO_3 and free lime CaO_l. And, the measured physical parameters are the LOl and the finesse (refusal at 80 microns).

For the mineralogical parameters which characterize the quality of the clinker are silica modules: The alite C_3S, the belite C_2S, the calcium aluminate C_3A and the aluminoferrite C_4AF. It is in total 17 parameters which are the endogenous variables (inputs) of the model multilinear regression and they are developed for each cement according to: NM.10.01.004 [16] and the European standard EN 197-1 [17]. In this study, the number of the cements studied is 158 samples and the expected results of the model studied for resistance to compression at 2, 7 and 28 days, are the assessment parameters of the quality's cements CPJ_{55}. They are represented by y_2, y_7 and y_{28}, which are the exogenous variables of the model. Table 1 shows the format and the coding of the individual input and output variables.

Table 1: Coding of variables needed to build statistical models

Code	Input variables	Code	Output Variables
d_1	C_3S	y_2	CCS at 2 days
d_2	C_2S		
d_3	C_3A		
d_4	C_4AF		
d_5	SiO_2		
d_6	Al_2O_3	y_7	CCS at 7 days
d_7	CaO		
d_8	CaO_l		
d_9	Fe_2O_3		
d_{10}	SO_3	y_{28}	CCS at 28 days
d_{11}	MgO		
d_{12}	LOI		
d_{13}	refusal at 80µm		
d_{14}	% clinker		
d_{15}	% fly ash (FA)		
d_{16}	% gypsum		
d_{17}	% limestone		

Table 2 shows the average characteristics of the input and output parameters which are used in the models of the multilinear regression and they are corresponding to 158 sample.

Table 2: Average characteristics of input and output data of MLR models

	Variable	Minimum	Average	Maximum
Input variables	Clinker (KK)	65.84	82.92	97
	limestone	0	10.45	21.34
	gypsum	3	4.29	5.4
	Fly Ash (FA)	0	2.33	9.02
	MgO	1.15	1.46	2.49
	C_3A	6.73	7.53	8.55
	C_2S	5.1	16.86	23.6
	SO_3	0.9	1.64	2.5
	CaO_l	0.6	1.82	4.1
	C_3S	49.9	57.01	67.2
	C_4AF	8.6	10.57	12.2
	CaO	64.9	65.58	67.1
	SiO_2	19.4	20.85	21.7
	Al_2O_3	4.8	5.06	5.4
	Fe_2O_3	2.8	3.48	4
	LOI	0.1	0.16	0.91
	Refusal at 80µm (R_{80})	0.4	1.63	6.1
Output variables	CCS 2days	9.81	20.78	32.8
	CCS 7 days	17.46	32.93	48.50
	CCS 28 days	27.87	46.93	59.2

Establishment of the model equation of MLR

The equation of the multivariate regression linking the input variables (d_1, d_2, d_3, ..., d_{16}, d_{17}) to the output variable (y_2, y_7 and Y_{28}), and this equation is written in the form:

$$y_n = f\,(d_1, d_2, d_3, \ldots, d_{16}, d_{17})$$

With: n = 2, 7, 28 days.

The functions obtained by the MLR will be used to produce CS of the cements CPJ_{55} at 2, 7 and 28 days. The treatment of the stepwise regression data of all the constituents of the cement and the experimental results of the compressive strength at the different ages; was conducted by SPSS [18]. The latter provides an optimal functionality, flexibility and ease of use, which are not available with traditional statistical software [19] and it has the advantage of the control of the repeatability, the handling, the powerful and sophisticated analysis of complex data [20].

The execution of the downward MLR statistical processing of data, allowed to screen all input factors and to select those that have a significant effect on responses. The different combinations of these variables were selected to intuitively take into account all the variables in the global model, in order to eliminate one by one, those variables corresponding to the smallest value of the t Student test, represented by p-value (p-value < 0.05).

Accordingly, the algorithm of MLR selected among thindependent input variables, the one that provides the greatest reduction of the residual variance (unexplained) of the dependent variables. In other words, these variables have the highest partial correlation with the response y (**CCS** at 2, 7 and 28 days).

The coefficients corresponding to the CS models of the cements CPJ_{55} are listed in Table 3.

Table 3: Coefficients selected for the three models corresponding to CCS at different ages

	Model of the CCS in function of time								
Time (days)	**2**			**7**			**28**		
Input variables	**Coefficients**	**t**	**p-value**	**Coefficients**	**t**	**p-value**	**Coefficients**	**t**	**p-value**
Constant	-475.50	-2.97	0.004	-622.13	-1.61	0.000	-325.48	-2.96	0.004
$R_{80\mu m}$	-1.89	-8.05	0.000	-2.49	-10.63	0.000	-4.01	-18.14	0.000
MgO	7.19	3.77	0.000	9.49	4.98	0.000	4.62	2.88	0.005
limestone	-0.35	-4.67	0.000	-0.46	-6.16	0.000	-0.40	-5.45	0.000
SO_3	-7.42	-2.48	0.015	-9.79	-3.27	0.000	6.57	3.85	0.000
SiO_2	-31.07	-3.50	0.001	-41.01	-4.62	0.000	3.95	3.46	0.000
CaO	24.53	3.70	0.000	32.38	4.88	0.000	3.86	2.76	0.007
Al_2O_3	-28.36	-3.00	0.004	-37.44	-3.96	0.000	6.36	2.84	0.006
LOI	-	-	-	-	-	-	-15.08	-3.48	0.001
CaO_l	-20.50	-3.38	0.001	-27.06	-4.46	0.000	-	-	-
C_3S	-4.83	-3.46	0.001	-6.38	-4.57	0.000	-	-	-

Moreover, the results of the table 3 reports that the parameters estimation by the maximum likelihood reveals show there is nine variables (9) truly significant in the multivariate models for predicting **CCS** at 2 and 28 days also eight variables (8) for the model predicting **CCS** at 7 days, given the values of probability (p-value <0.05). Similarly, the SPSS shows in its 5th step of the 2 and 7 days models and in its 6th step of the 28 days model, that "no other variable can be deleted or added to the current model". Therefore, the algorithm model MLR removes systematically the variables whose its significance is too low, and compared to the resistance of 2 to 28 days at each stage. And the non-selected variables in the three models for each 4 steps are shown in Table 4.

Table 4: Variables excluded in the three models

Step	variables deleted	Model of CCS in function of time (days)					
		2		7		28	
		t	p-value	t	p-value	t	p-value
1	KK	-0.504	0.616	-0.66	0.81	-0.868	0.388
	C_3A	1.103	0.274	1.45	0.362	-0.016	0.988
	C_2S	1.079	0.284	1.42	0.375	-1.083	0.282
	C_4AF	-1.107	0.272	-0.09	0.36	0.019	0.985
2	LOI	-0.128	0.898	-0.17	1.185	-	-
	CaO_l	-	-	-	-	0.035	0.972
3	Fe_2O_3	-1.106	0.272	-1.46	0.36	0.567	0.572
	FA	0.526	0.600	0.069	0.79	-	-
4	C_3S	-	-	-	-	1.244	0.217
	gypsum	1.001	0.320	1.321	0.422	-	-
5	Fe_2O_3	-1.106	0.272	-1.46	0.36	-	-
	FA	-	-	-	-	1.352	0.181
6	gypsum	-	-	-	-	-1.561	0.123

Statistical model validation tests

The model validation was carried out by the coefficients of multiple determination tests R^2, Fisher and the Durbin-Waston test, which were calculated from the data indicated in the table of the multivariate analysis of variance (MANOVA)[21] (Table 5). The data results of the three tests are significant at the 5th stage for the 2 and 7 days model and at 6th stage for 28 days model, because that the R-squared (R^2) values are 95.3; 97.1 and 98.1%, respectively. So we conclude that the global significance of the models is good. Thus, the resulting models have excellent predictive qualities (Table 6).

Table 5: MANOVA data

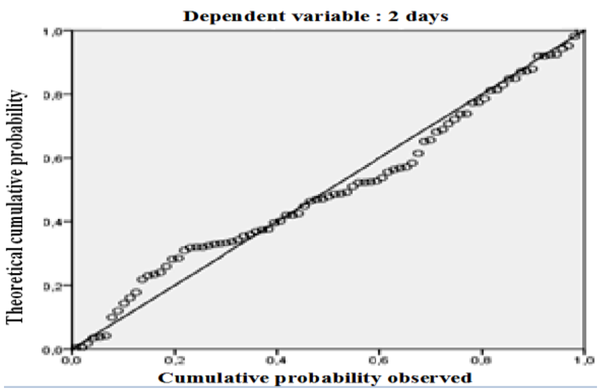
	Time (days)	Model of CCS in function of time					
		2		7		28	
	Model	**F**	**p-value**	**F**	**p-value**	**F**	**p-value**
1	Regression	37.979	0.000	50.132	0.000	146.886	0.000
2	Regression	41.712	0.000	55.43	0.000	161.364	0.000
3	Regression	45.934	45.934	60.63	0.000	177.656	0.000
4	Regression	50.43	0.000	66.56	0.000	193.831	0.000
5	Regression	55.73	0.000	73.56	0.000	212.82	0.000
6	Regression	-	-	-		234.68	0.000

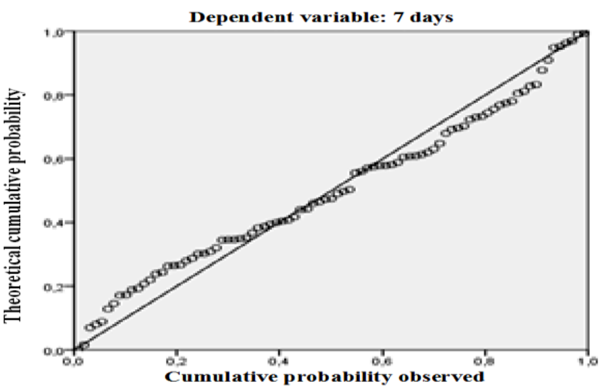
The variation of Fisher test associated to the three models is significant (p-value <0.001). Therefore, these models explain a significant proportion of the variables variance of CCS of the CPJ_{55} at 2, 7 and 28 days.

Table 6: Statistical model Validation Data

Measurement time of the CS	Model	R^2	Standard error of the estimate	Variation of F	Sig. Variation of F	Durbin-Watson
2	1	0.935	2.16	37.979	0.000	2.47
	2	0.935	2.14	0.016	0.78	
	3	0.935	2.13	0.277	0.71	
	4	0.934	2.13	1.001	0.41	
	5	0.933	2.14	1223	0.30	
7	1	0.973	2.86	38.66	0.000	2.21
	2	0.973	2.84	0.008	0.928	
	3	0.973	2.82	0.070	0.793	
	4	0.973	2.81	0.48	0.490	
	5	0.971	2.83	215	0.147	
28	1	0.982	1.89	146.886	0.000	1.85
	2	0.982	1.88	0.001	0.972	
	3	0.982	1.87	0.322	0.572	
	5	0.981	1.88	1.548	0.217	
	6	0.981	1.89	1.828	0.123	

As for the test of the Durbin-Watson, there is no associated significance. For the **CCS** prevention models at 2, 7 and 28days, the value of the statistic that is acceptable, are 2.47; 2.21 and 1.85, respectively, because they are between 1 and 3 [2] and close to the value of 2. This saves there are fewer problems in terms of independence errors [22,23]. So, the independence and the normality of these residues are proved by the analysis of the right of Henry (Fig.1) which allowed us to note that the observed distribution of residues of the three models is strongly adjusted to the normal law because the linearity is satisfactory; this proves the good quality of the sampling.





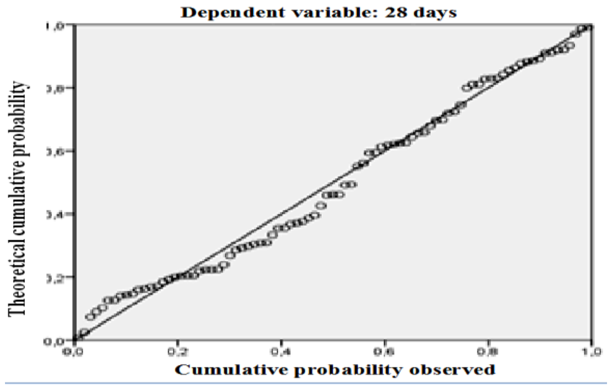


Figure 1: straight Henry standardized residues of cement CPJ55 models at 2, 7 and 28 days

The analysis of the Fisher test's results F (Table 6) showed that the developed models are very significant. Indeed, the models values of the **CCS** at 2 to 28 days are 55.73; 73.56 and 234.68 respectively, and they are significant at p-value <0.001. This indicates that we have less than 0.1% chance of being wrong in claiming that the models contribute to better predict the CS and the level of significance is the best. Accordingly, the three equations of the regression are very good and record that the variables forming the prediction equation of the CS at 2, 7 and 28 days contribute in a very reproducible way in the **CCS** variable score at 2, 7 and 28 days while providing a significant amount of information to models with a maximum error of the data is about **2.14; 2.83 and 1.89**.

The functions generated by the algorithm MLR presenting the best result for predicting **CCS** of CPJ55 at 2, 7 and 28 days according to the chemical and mineralogical composition of the clinker are given by equations (1), (2) and (3).

$$\begin{aligned} y_{2days} = {} & -475{,}50 + 7{,}19\mathbf{MgO} - 1{,}89\mathbf{R_{80}} - 0{,}35\mathbf{limestone} - 7{,}42\mathbf{SO_3} - 31{,}07\mathbf{SiO_3} \\ & + 24{,}53\mathbf{CaO} - 28{,}36\mathbf{Al_2O_3} - 20{,}50\mathbf{CaOl} \\ & - 4{,}83\mathbf{C_3S} \qquad\qquad (1) \end{aligned}$$

$$\begin{aligned} y_{7days} = {} & -622{,}13 - 6{,}38\mathbf{C_3S} - 2{,}49\mathbf{R_{80}} + 9{,}49\mathbf{MgO} - 0{,}46\mathbf{limestone} - 9{,}79\mathbf{SO_3} \\ & - 41{,}01\mathbf{SiO_2} + 32{,}38\mathbf{CaO} - 37{,}44\mathbf{Al_2O_3} \\ & - 27{,}06\mathbf{CaO_l} \qquad\qquad (2) \end{aligned}$$

$$\begin{aligned} y_{28days} = {} & -325{,}48 - 4{,}01\mathbf{R_{80}} + 4{,}62\mathbf{MgO} - 0{,}40\mathbf{limestone} + 6{,}57\mathbf{SO_3} + 3{,}95\mathbf{SiO_2} \\ & + 3{,}86\mathbf{CaO} + 6{,}36\mathbf{Al_2O_3} \\ & - 15{,}08\mathbf{LOl} \qquad\qquad (3) \end{aligned}$$

Experimental validation of models

Model validation of compressive strengths of the cements CPJ55 at 2, 7 and 28 days was conducted by established experimental development of 30 mortar cements according to the standards NM.10.01.004 [16] and the European standard EN 196-1, and those cements were tacked directly from the cement Doser of the cement CPJ55. The physico-chemical and mineralogical composition of the various components has been performed in the laboratory of the company Asment Temara according to standard NM.10.01.005 [13].

The results of the validation test of the three functions are shown in Figures 2 to 4. The compressive strengths of the cement CPJ55 at different ages were measured experimentally for 30 days, corroborate to those calculated and predicted theoretically from the three models established by multiple regression. So the three functions of the MLR are able to present the real value of the compressive strength with the minimal error.

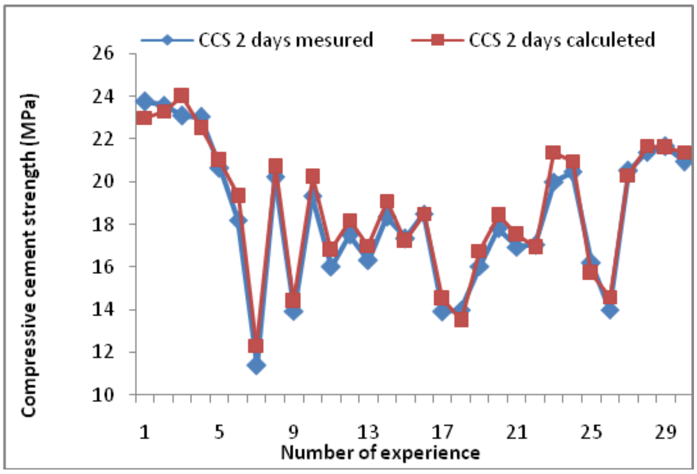


Figure 2: Evaluation of MLR model for predicting resistance of 30 trying of the cements CPJ_{55} at 2 days

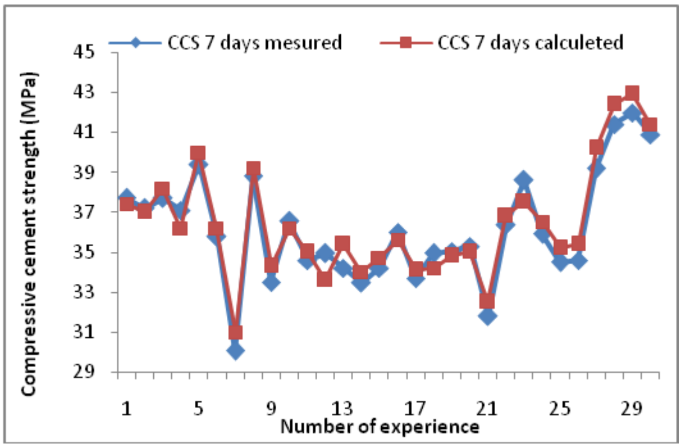


Figure 3: Evaluation of MLR model for predicting resistance of 30 trying of the cements CPJ_{55} at 7 days

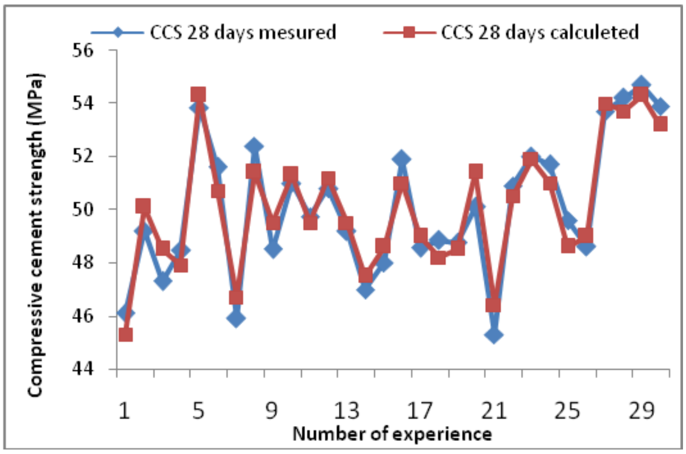


Figure 4: Evaluation of MLR model for predicting resistance of 30 trying of the cements CPJ_{55} at 7 days

The results presented in Figures 2, 3 and 4 show that the variability explained by models 1, 2 and 3 is good, since the calculated differences between the compressive strength calculated from the established mathematical equations and those measured by the traditional method is always less than **2.14; 2.83 and 1.89** for model 2, 7 and 28 days, respectively. So, the three models are experimentally reliable and predictive.

ISSN: 0975-8585

CONCLUSION

In this study, three multilinear regression models were developed for prediction the compressive strength of the cement CPJ_{55} at 2, 7 and 28 days, according to the chemical and mineralogical composition of its constituents (limestone, clinker, gypsum and fly ash). The analysis of the MLR has shown that these models have a high predictive power of the resistance from the combination of effects of the selected factors. Similarly, the effects of these factors Al_2O_3, Fe_2O_3, CaO_l, C_2S, SiO_2, SO_3, CaO, % fly ash, % clinker, %gypsum, including the size distribution of the cement grains, were modelled to have the models with the least errors.

Feasibility tests of these models in the industrial scale revealed that the operated models are developers and they have useful tools to prevent the compressive strength of cement at any age.

This study will be helping the industry to:

- Minimize the clinker rate used,
- Minimize CO_2 emissions
- Cement production cost while maintaining the same quality of the cement CPJ_{55}
- Reduce the energy consumption
- Conserve natural resources.

REFERENCES

[1] Akkurt S., Ozdemir S., Tayfur G., Akyol B., Cem. Concr, Res. 33 (2003) 973.
[2] Rakotomalala R., PhD thesis, University of Lyon (Lyon, France, 2011).
[3] Akkurt S., Ozdemir S., Tayfur G., Trans C., Miner. Process. Extr. Metall. 12 (2003) 1.
[4] Liang G.F., Cem. Concr. Res. 37 (2007) 1003.
[5] Baykasoglu A., Dereli T., Tanıs S., Cem. Concr. Res. 34 (2004) 2083.
[6] Mtarfi N.H., Rais Z., Saffaj T., Kada K.M., *IJIAS.* 10 (2015) 1291.
[7] Tsivilis S., Parissakis G., Cem. Concr. Res. 36 (2005) 998.
[8] De Siquera Tango C.E., Cem. Concr. Res. 39 (2008) 1069.
[9] Wang J.Z., Ni H.G., Cem. Concr. Res. 30 (2000) 1245.
[10] Jacquard J., Turrisi R., PhD thesis, Sage University (Ivrine, United States, 2003).
[11] Ferreira C., Complex. Syst. 27 (2001) 87.
[12] Saporta G., J. Technip. 2 (2006) 267.
[13] Moroccan Industrial Standards Service (SNIMA), Standard Moroccan, 3 (2008) 120.
[14] European Committee for Standardization (CEN), AFNOR, 2 (2006) 202.
[15] Kahya E., Appl. Math. Comp. 2 (2005) 912.
[16] Moroccan Industrial Standards Service (SNIMA), Standard Moroccan, 4 (2003) 24.
[17] European Committee for Standardization (CEN), AFNOR, 1 (2000) 243.
[18] Ergu¨n M., JAAH, 5 (1995) 422.
[19] Verlen J., SPSS. 8 (2009) 287.
[20] Besse P., PhD thesis, Paul Sabatier University (Toulouse, France, 2003).
[21] Huberty C., Olejnik J.S., Hoboken, New Jersey: John Wiley and Sons, Inc. 2 (2006) 309.
[22] I. Cadoret, PhD thesis, Oxford University (Oxford, Royaume-Uni, 2004).
[23] Veysseyre R., Statistics and Probability for Engineers, DUNOD**,** Aide memoire of the engineer, 3 (2014) 187.