Prediction of Concrete Properties Using Coarse Aggregate Chemical Composition Data

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Regression models that predict the compressive strength, tensile strength, modulus of elasticity, and drying shrinkage of concrete made with several coarse aggregates are presented in this paper. The findings are part of a comprehensive research study being conducted in Texas for determining the effect of aggregates on the performance of concrete pavements. Using statistical analysis of laboratory test data from concrete samples made with eight commonly used aggregates of known chemical composition, regression models were developed to predict the concrete properties just mentioned. The predicted values were then compared with the laboratory test results, and the models were used to predict the concrete properties of 11 additional untested coarse aggregates also used for pavement construction in Texas. The predicted concrete properties were within the pavement concrete range reported for these types of concrete mixtures. These prediction models can estimate preliminary information for coarse aggregates or coarse aggregate blends from chemical composition data before casting and testing of concrete samples. This will allow for initial screening of proposed new sources of coarse aggregate or tentative blends of new or existing aggregate sources of known chemical composition.

In portland cement concrete (PCC) pavement construction, the importance of using the right type and quality of aggregate cannot be overemphasized because the fine and coarse aggregates occupy roughly 60 to 75 percent of the concrete volume (70 to 80 percent by weight) (*1*). For given environmental conditions, changes in concrete volume stresses depend on modulus of elasticity, thermal properties, and drying shrinkage of the concrete. These concrete properties, as well as wheel load stresses, depend on the tensile strength and modulus of the concrete, which in turn depend largely on the type of coarse aggregate used (*2*). In PCC pavement design, most states do not consider coarse aggregate type as a design variable. However, field observation has shown significant variation in the performance of pavements built with different coarse aggregates (*3*).

The findings reported in this paper are part of results from a comprehensive research study being conducted by the Center for Transportation Research (CTR) of The University of Texas at Austin for the Texas State Department of Highways and Public Transportation (SDHPT) to determine the effects of aggregate types on the performance of concrete pavements.

The Texas SDHPT has recently taken steps to recognize the influence of coarse aggregate type on the performance of concrete pavements. SDHPT has developed PCC pavement designs that incorporate these effects to provide equal performance of pavements made with any type of coarse aggregate (*4*). The large number of aggregate sources in the state that are approved for concrete pavement construction make this consideration important. Sand and siliceous river gravel; limestone; to some extent, granite, basalt, and sandstones; and blends of these aggregates can be used for the construction of concrete pavements in Texas.

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OBJECTIVE, APPROACH, AND SCOPE

The objective of this paper is to present the Texas SDHPT approach for fast and simple assessment of pavement concrete properties that can be used with appropriate pavement design procedures. The advantage of this technique is that by using a surrogate test such as the chemical analysis of the coarse aggregate (chemical and mineral composition of the aggregate can be obtained, in most cases, directly from the supplier), one can quickly estimate preliminary concrete properties versus age before expensive laboratory testing. This permits the initial evaluation of proposed new sources of coarse aggregate or blends and can also be used to predict the current performance of aggregates such as limestone, which is quarried from bedded strata and thus may vary significantly in chemical composition, even when quarried from the same source.

The approach taken in this study was to develop regression models for predicting 28-day (256 days for shrinkage) concrete properties from the chemical makeup of the coarse aggregate used to produce the concrete. These models were developed with laboratory test data from concrete made with eight carefully chosen coarse aggregates representing the wide range of aggregates used in Texas pavements.

The interdependence, or correlation, that exists among the various chemical components of the coarse aggregates was determined using chemical composition data from 20 different aggregate types. Once the 28- (or 256-) day models were developed, two models (Models 1 and 2) were proposed to predict the concrete properties at any age using the 28- or 256-day value and the curing age as the sole input.

These prediction equations are limited to modeling properties of concrete mixes made with Type I cement cured at 75°F and 40 percent relative humidity. These curing conditions were chosen to simulate field curing in pavements. The predictions may not be applicable to concrete mixtures made with other types of cement and cured under other conditions.

All of the aggregates tested conform to SDHPT Specification 360. This ensured adequate grading and reduced any effect of aggregate shape. No deleterious aggregates were used, and the models are not intended to predict for them.

TEST RESULTS

Laboratory test results of concrete specimens made with eight different coarse aggregates were obtained using standard ASTM procedures as follows:

Laboratory Property	*ASTM Standard*	*Curing Conditions* °F	*Humidity (%)*	*Curing Time (days)*
Compressive strength	C 39	75	40	1, 3, 7, 28
Tensile strength	C 496	75	40	1, 3, 7, 28
Modulus of elasticity	469	75	40	1, 3, 7, 28
Drying shrinkage	None	75	40	1 through 256

Chemical composition data were obtained for coarse aggregates from 20 different sources using X-ray diffraction, fusion, and coulometric techniques (*5*). The major chemical components of eight commonly used aggregates are reported in Table 1. These aggregates were also used to obtain the pavement concrete properties just listed. The X-ray diffraction results of all aggregates used as part of this study for which chemical composition data were available are presented in Table 2.

DATA ANALYSIS METHODOLOGY

It is generally accepted that the curing rate of concrete depends primarily on the type of cement used and the temperature and humidity conditions experienced during curing (*6*). The use of different types of coarse aggregate, therefore, has the greatest effect on the final strength of the concrete. Because all the concrete specimens cast for this study were mixed and cured identically, any differences (excluding normal material variances, laboratory test repeatability, etc.) in the final properties can be attributed to aggregate influence, with curing rates being similar for all specimens (*7*).

Estimating concrete properties from coarse aggregate chemical composition data was therefore a two-step process. The first phase of the analysis consisted of developing models for predicting 28-day concrete properties from chemical composition. Because drying shrinkage develops more slowly, and because long-term shrinkage data were available for 256-day cured specimens, these long-term values were used in the analysis instead of the 28-day values.

CONCRETE PROPERTIES AT 28 DAYS

Because concrete properties were tested for only the eight aggregates listed in Table 1, there are insufficient degrees of freedom to use all 10 chemical components or their interactions in a standard analysis of variance (ANOVA). A correlation analysis was run instead, as a preliminary step, using the Pearson product-moment correlation (*8*) to determine which chemicals were interdependent or correlated with one another. All 20 aggregates were used to determine these chemical associations. The results indicated that the chemicals belong to the following groups, probably as they exist naturally as ores:

Group 1	*Group 2*	*Group 3*	*Group 4*	*Group 5*
SiO_2	CaO	MgO	Fe_2O_3	Al_2O_3
	CO_2		MnO	TiO_2
				Na_2O
				K_2O

Further examination of the chemical data revealed a strong negative correlation between Groups 1 and 2, indicating that whenever SiO_2 is present in high concentrations, CaO and CO_2

TABLE 1 COARSE AGGREGATE CHEMICAL ANALYSIS DATA

Source	Aggregate Type		SiO_2	CaO	MgO	CO_2	MnO	Fe_2O_3	Al_2O_3	Na_2O	K_2O	TiO_2	Other
McCelligan	Dolomite	(DL)	6.53	34.9	13.0	42.9	.02	0.21	0.38	0.09	0.26	0.02	1.69
Western-T	S/L	(WT)	68.5	11.4	0.35	8.98	.05	2.64	3.97	0.85	1.1	0.17	1.99
Bridpt+TinTop	L+S/L	(BTT*)	17.53	42.55	0.71	35.65	0.04	0.57	0.56	0.15	0.30	0.04	1.91
Feld (TCS)	Limestone	(LS)	2.56	45.7	5.97	43.3	.01	0.06	0.21	0.14	0.21	0.02	1.82
Fordyce	SRG	(SRG)	93.8	2.23	0.11	1.77	.01	0.76	0.63	0.18	0.32	0.1	0.09
Vega	SRG	(VG)	66.9	11.6	0.39	9.07	.07	2.33	4.22	0.95	1.16	0.19	3.12
Ferris	L/S	(FR)	14.2	42.1	0.43	34.4	.10	3.70	0.87	0.17	0.26	0.06	3.71
Scotland	Granite	(GR)	71.3	1.5	0.63	0.59	.03	1.52	14.3	4.4	3.83	0.29	1.61
TXI-Boonesville		(BO)	5.26	49.8	0.34	40.0	0.03	0.40	0.41	0.06	0.14	0.02	3.54
McCelligan Canyon #2		(DL2)	7.31	35.2	12.4	42.8	0.02	0.21	0.42	0.11	0.29	0.03	1.21
Ferris #2		(FR2)	12.5	42.8	0.44	35.4	0.10	3.56	0.76	0.17	0.28	0.06	3.93
TCP-Cleburne #51		(CL)	18.8	41.3	0.49	34.7	0.05	0.72	0.62	0.19	0.31	0.04	2.78
Ingram Whitehead		(IW)	23.9	38.7	0.44	31.2	0.05	0.77	0.69	0.21	0.32	0.05	3.67
TXI-Tin Top #2		(TT2)	33.6	34.1	0.35	27.9	0.06	0.91	0.74	0.16	0.32	0.05	1.81
Pioneer-Landess Pit		(PI)	14.7	42.8	0.42	34.7	0.09	3.31	0.65	0.15	0.25	0.05	2.88
Jobe-Hueco		(JH)	17.5	41.7	1.62	35.1	0.02	0.45	1.01	0.16	0.35	0.06	2.03
Rainbow-Baker Pit		(RB)	32.8	34.6	0.41	27.9	0.06	0.98	0.69	0.21	0.36	0.05	1.94
A-Rock Brazos River Pit		(BR)	55.6	20.2	0.43	16.4	0.03	0.89	2.31	0.64	0.93	0.11	2.46
Vulcan-Mexico		(VM)	0.27	53.1	0.55	43.8	0.01	0.03	0.23	0.18	0.28	0.04	1.51

* These aggregates combined in a 50/50 blend when tested in the laboratory for concrete properties.

TABLE 2 MINERALOGICAL RESULTS (X-RAY DIFFRACTION)

		Minerals Found		
Source	Aggregate Type	Most Abundant	Second	Third
McCelligan Canyon # 1	DL	Dolomite	Calcite	Quartz
Western-Tascosa	WT	Quartz	Calcite	
Tin-Top # 1	BTT	Calcite	Quartz	
Bridgeport	BTT	Calcite	Dolomite	Quartz
Feld (TCS)	LS	Calcite	Dolomite	Quartz
Fordyce	SRG	Quartz	Calcite	
Vega	VG	Quartz	Calcite	
Ferris # 1	FR	Calcite	Quartz	
Scotland Granite	GR	Quartz	Albite	
TXI-Boonesville	BO	Calcite	Quartz	
McCelligan Canyon # 2	DL2	Dolomite	Calcite	Quartz
Ferris # 2	FR2	Calcite	Quartz	
TCP-Cleburne # 51	CL	Calcite	Quartz	
Ingram Whitehead	IW		Calcite	Quartz
TXI-Tin Top # 2	TT2	Calcite	Quartz	
Pioneer-Landerss Pit	PI	Calcite	Quartz	
Jobe-Hueco	JH	Calcite	Quartz	
Rainbour-Baker Pit	RB	Calcite	Quartz	
A-Rock Brazos River Pit	BR	Calcite	Quartz	
Vulcan-Mexico	VM	Calcite	Quartz	

are not present in an aggregate. It would therefore be unnecessary to include both groups in the statistical analysis. On the basis of these observations, only Groups 2 through 5 were selected as regressors, using the compound present in highest concentration to represent each group. Thus CaO, MgO, Fe_2O_3, and Al_2O_3 were selected as primary regressors. CaO was chosen over CO_2 because a portion of the CO_2 was released from $CaMg(CO_3)_2$ (dolomite) during the high-temperature analysis. This was confirmed by the partial positive correlation between CO_2 and MgO observed in the analysis.

REGRESSION MODELS FOR 28-DAY CONCRETE PROPERTIES

Using the four primary regressors selected and their two-way interactions, a stepwise regression (*8*) was used to determine the best models for 28-day tensile strength, compressive strength, modulus of elasticity, and 256-day drying shrinkage. Drying shrinkage was predicted at 256 days because laboratory measurements were available for all eight tested aggregates at that time. Models were restricted to three or fewer predictors to avoid the artificially high R^2 (and consequent low predictive ability) associated with models with few degrees of freedom (*9*). Calculating regression coefficients resulted in the following models:

$$f_c(28) = -403.2 \cdot \ln(\text{CaO}) + 6.806\,(\text{CaO}/\text{Al}_2\text{O}_3) + 5{,}120.5 \qquad (1)$$

$$f_t(28) = -59.238 \cdot \ln(\text{CaO}) + 46.884 \cdot \ln(\text{MgO}) + 1.7159\,(\text{CaO}/\text{MgO}) + 572.2 \qquad (2)$$

$$E(28) = -0.4135 \cdot \ln(Al_2O_3) + 0.264 \cdot \ln(MgO) - 0.00948\,(CaO/Al_2O_3) + 4.664 \quad (3)$$

$$Z(256) = 1.8723\,(CaO \cdot Al_2O_3) + 0.1223\,(CaO/Fe_2O_3) - 0.1383\,(CaO \cdot MgO) + 350.6 \quad (4)$$

where

$f_c(28)$ = 28-day concrete compressive strength (psi),
$f_t(28)$ = 28-day concrete tensile strength (psi),
$E(28)$ = 28-day concrete modulus of elasticity (10^6 psi), and
$Z(256)$ = 256-day concrete drying shrinkage (in./in. 10^{-6}).

Scattergrams showing the predicted 28- (or 256-) day pavement concrete properties obtained using Equations 1–4 versus laboratory results are given in Figures 1–4. As shown in these graphs, the average laboratory test values can be accurately predicted using the equations.

TIME-DEPENDENT MODELS OF CONCRETE PROPERTIES

After the 28-day models had been developed, the second phase was to determine a method to estimate the pavement concrete properties for any given curing time, t. If concrete curing time is assumed to be independent of coarse aggregate type, all that is needed is to calculate a normalized curing curve for each of the material properties, adjusting it for each aggregate using the 28-day (256-day, for Z) values predicted by Equations 1–4. Although four curing models were developed, only the best two are presented.

Model 1

The American Concrete Institute (ACI) Committee 209 proposed the following model expressing compressive strength

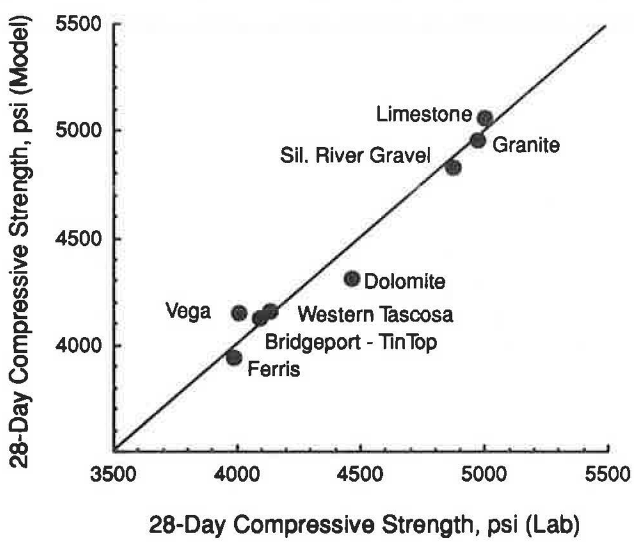

FIGURE 1 Predicted versus actual compressive strength.

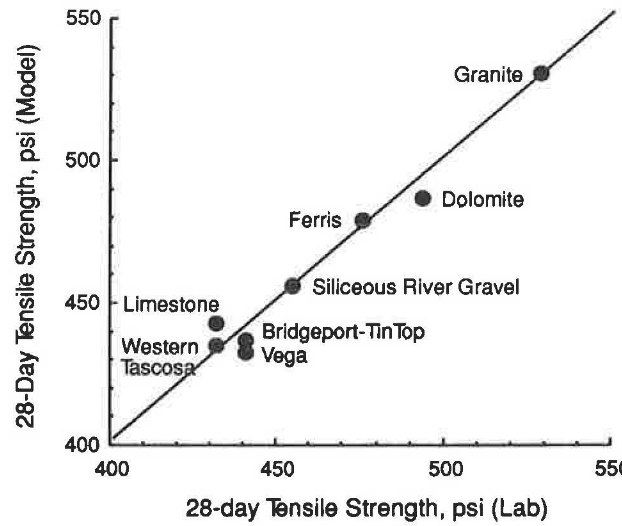

FIGURE 2 Predicted versus actual tensile strength.

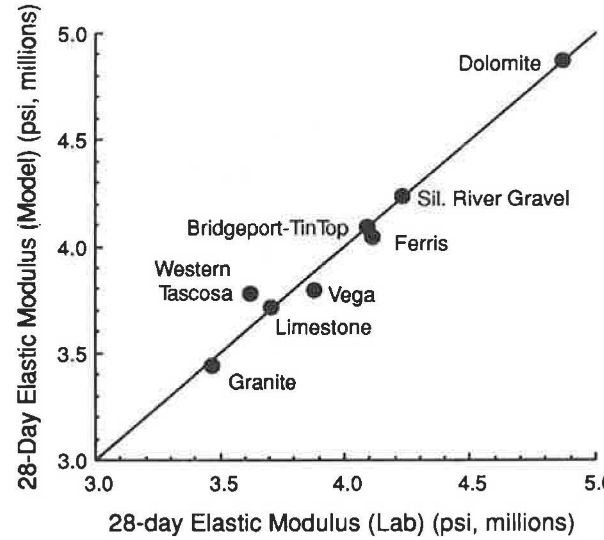

FIGURE 3 Predicted versus actual modulus of elasticity.

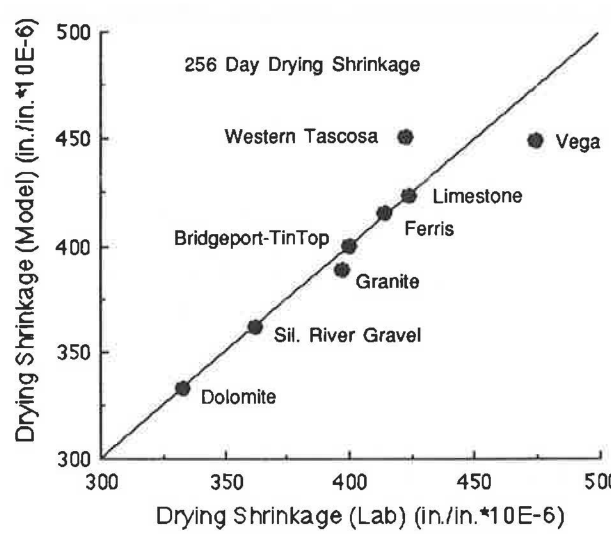

FIGURE 4 Predicted versus actual drying shrinkage.

at time t as a percentage of the 28-day compressive strength for Type I cement moisture cured at 70°F (*10*):

$$f_c(t) = f_c(28)\cdot\left(\frac{t}{4 + 0.85t}\right) \quad (5)$$

In the general form, this equation becomes

$$F(t) = F(28)\cdot\left(\frac{t}{A + Bt}\right) \quad (6)$$

where F is the concrete property function (f_c, f_t, E, or Z) at time t, and A and B are coefficients of curvature, which can be determined by regression. The following time-dependent curves were obtained, averaged for all aggregates:

$$f_c(t) = f_c(28)\cdot\left(\frac{t}{2.1743 + 0.90597t}\right) \quad (7)$$

$$f_t(t) = f_t(28)\cdot\left(\frac{t}{(1.43139 + 0.94156t}\right) \quad (8)$$

$$E(t) = E(28)\cdot\left(\frac{t}{0.43056 + 0.99451t}\right) \quad (9)$$

$$Z(t) = Z(256)\cdot\left(\frac{t}{23.851 + 0.91056t}\right) \quad (10)$$

Model 2

The second successful model form is adapted from one of the prediction equations proposed by CTR research studies (*11*):

$$F(t) = F(28)(A)\cdot(2 - e^{-Bt} - e^{-Ct}) \quad (11)$$

Again, combining concrete property data from all eight aggregates and finding a least-squares fit for A, B, and C, the following property curves were developed:

$$f_c(t) = f_c(28)\cdot(0.50136)\cdot(2 - e^{-0.57677t} - e^{-0.17658t}) \quad (12)$$

$$f_t(t) = f_t(28)\cdot(0.50189)\cdot(2 - e^{-0.19901t} - e^{-1.0597t}) \quad (13)$$

$$E(t) = E(28)\cdot(0.89032)\cdot(2 - e^{-0.004799t} - e^{-1.5282t}) \quad (14)$$

$$Z(t) = Z(256)\cdot(0.52452)\cdot(2 - e^{-0.067464t} - e^{-0.00984t}) \quad (15)$$

Typical curves predicted by Models 1 and 2 are plotted with laboratory data in Figure 5 for compressive strength of concrete (Equations 7 and 12) made with siliceous river gravel as the coarse aggregate, in Figure 6 for tensile strength of concrete (Equations 8 and 13) made with limestone as the coarse aggregate, in Figure 7 for modulus of elasticity of concrete (Equations 9 and 14) made with granite as the coarse aggregate, and in Figure 8 for drying shrinkage of concrete (Equations 10 and 15) made with siliceous river gravel as the coarse aggregate.

Typical predicted values for coarse aggregates that had undergone chemical analysis but not concrete testing are presented in Figure 9 for compressive strength of concrete (Equations 7 and 12) made with limestone/siliceous coarse aggregate (see also Table 2), in Figure 10 for tensile strength of concrete

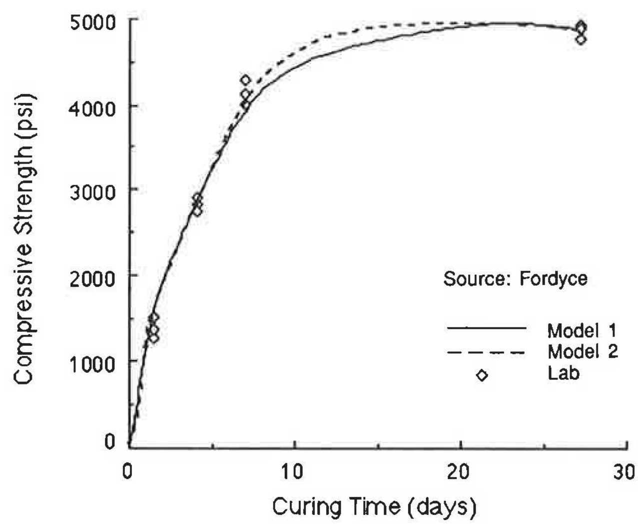

FIGURE 5 Predicted and laboratory compressive strength for PCC made with siliceous river gravel.

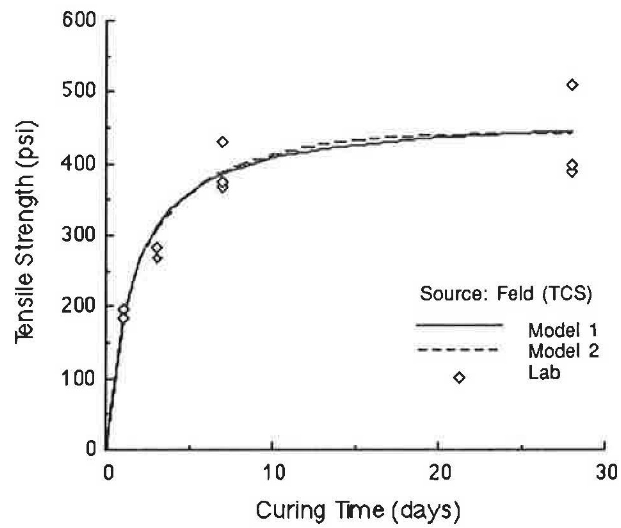

FIGURE 6 Predicted and laboratory tensile strength for PCC made with limestone.

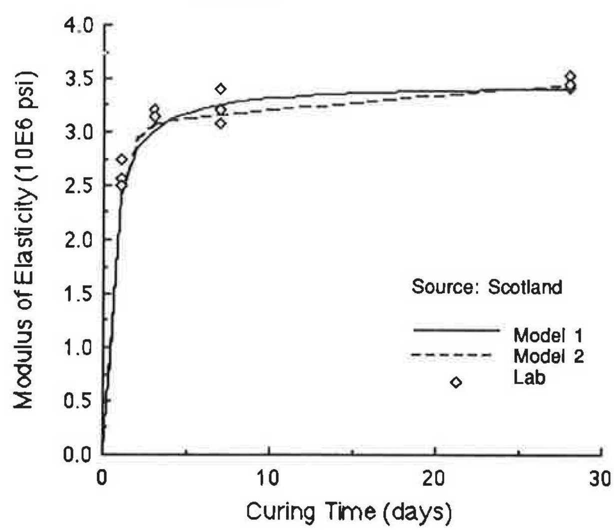

FIGURE 7 Predicted and laboratory modulus of elasticity for PCC made with granite.

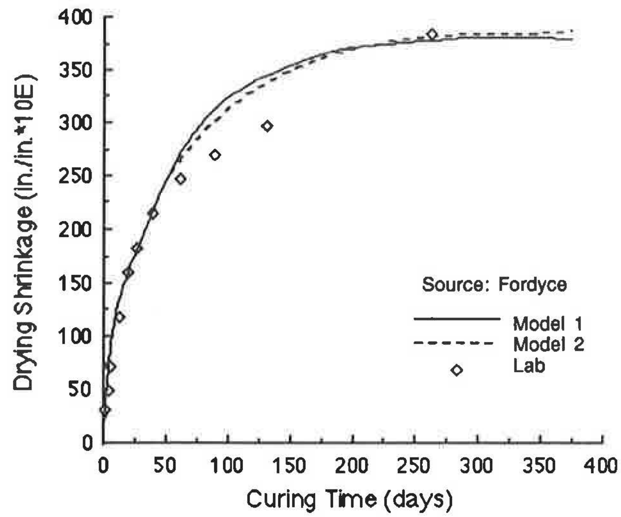

FIGURE 8 Predicted and laboratory drying shrinkage for PCC made with siliceous river gravel.

(Equations 8 and 13) made with dolomite coarse aggregate, in Figure 11 for modulus of elasticity of concrete (Equations 9 and 14) made with siliceous river gravel coarse aggregate, and in Figure 12 for drying shrinkage of concrete (Equations 10 and 15) made with Mexican limestone coarse aggregate.

CONCLUSIONS

Pavement concrete strength, modulus of elasticity, and drying shrinkage for curing times can be predicted accurately up to 28 days (256 days for shrinkage) using either Model 1 or 2, as demonstrated in Figures 5 through 8. The results from Models 1 and 2 are similar, each providing a reasonable fit, well within the normal material and testing variability demonstrated by the three replicate laboratory data points. In addition, Figures 9 to 12 show reasonable curves for PCC made with coarse aggregates not yet tested in the laboratory for concrete properties. Pavement concrete properties were

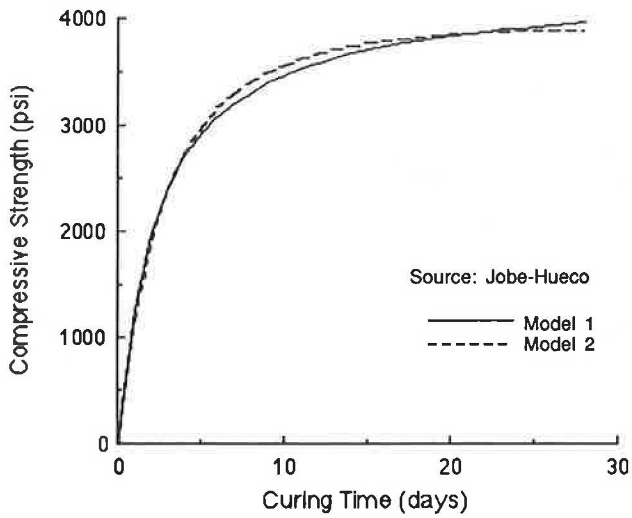

FIGURE 9 Predicted compressive strength for PCC made with limestone-siliceous aggregate.

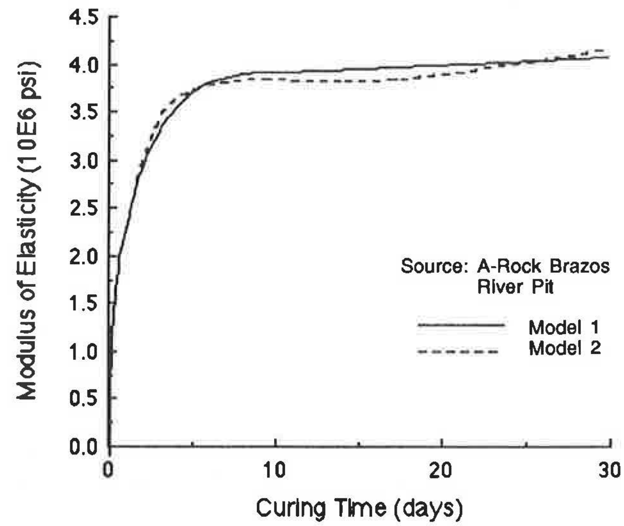

FIGURE 11 Predicted modulus of elasticity for PCC made with siliceous river gravel.

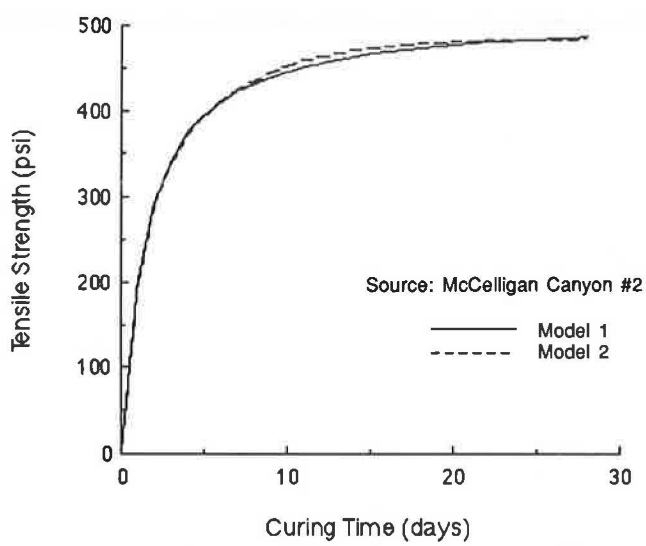

FIGURE 10 Predicted tensile strength for PCC made with dolomite.

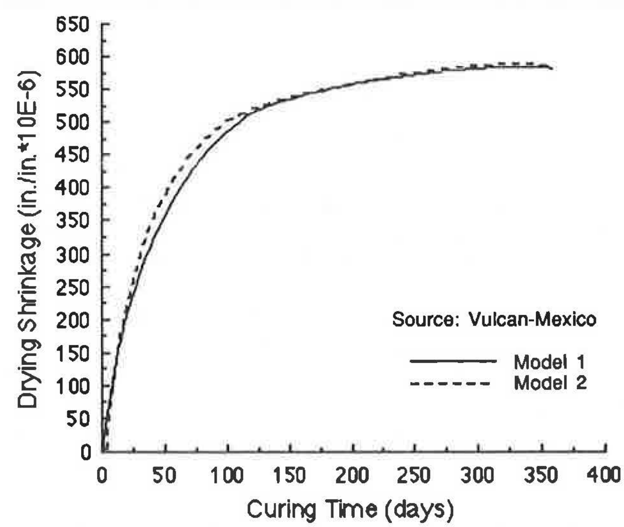

FIGURE 12 Predicted drying shrinkage for PCC made with limestone.

predicted approximately as reported by the suppliers of coarse aggregate (*8*), despite the wide variation in chemical composition and mineralogy of the aggregates investigated (see Tables 1 and 2).

RECOMMENDATIONS

If carefully applied within the inference space of the models (Table 3), either Model 1 or 2 can be used as given to provide a fast and inexpensive preliminary assessment of aggregate performance. Chemical composition data can often be obtained directly from the aggregate supplier. Of course, it is recommended that standard highway department test procedures be followed before any final decision is made regarding aggregate suitability.

Because laboratory testing has been conducted on only eight aggregates to date, testing of additional aggregates should improve the fit and expand the inference space of the model. Other interested organizations can use the approach and procedures outlined here to develop models for the cement types and aggregates of interest to them. For convenience in applying the models presented here, an interactive computer program, CHEM, for IBM PCs and compatibles has been prepared and is available from the authors.

TABLE 3 PERCENTAGE OF CHEMICAL COMPONENTS

	Range	
Compound	High	Low
SiO_2	93.8	2.56
CaO	45.7	1.50
MgO	13.0	0.11
Co_2	42.9	0.59
MnO	0.1	0.01
Fe_2O_3	3.7	0.06
Al_2O_3	14.3	0.21
Ma_2O	4.4	0.09
K_2O	3.8	0.21
TiO_2	0.29	0.02
Other	3.71	0.09

ACKNOWLEDGMENTS

The authors are pleased to acknowledge the support of the Center for Transportation Research, University of Texas at Austin, and the sponsor of the main study, the Texas Department of Highways and Public Transportation, in cooperation with the U.S. Department of Transportation, Federal Highway Administration. The assistance of Jian Lu and Bryan Black is gratefully acknowledged.

REFERENCES

1. S. H. Kosmatka and W. C. Panarese. *Design and Control of Concrete Mixtures*, 13th ed. Portland Cement Association, Skokie, Ill. 1988.
2. D. F. Orchard. *Concrete Technology, Vol. 1: Properties of Materials*, 4th ed. Applied Science Publishers, London, 1979.
3. M. Guiterrez de Velasco and B. F. McCullough. *Summary Report for 1978 CRCP Condition Survey in Texas*. Report 177-20. Center for Transportation Research, University of Texas at Austin, Jan. 1981.
4. M. C. Won. *Mechanistic Analysis of Continuously Reinforced Concrete Pavements Considering Materials Characteristics, Variability and Fatigue*. Ph.D. dissertation. Department of Civil Engineering, University of Texas at Austin, May 1989.
5. T. Dossey. *Prediction of Concrete Properties from Aggregate Chemical Assay*. Tech Memo 422-58. Center for Transportation Research, University of Texas at Austin, May 5, 1989.
6. J. G. MacGregor. *Reinforced Concrete: Mechanics and Design*. Prentice-Hall, Eaglewood Cliffs, N.J., 1988.
7. H. Castedo. *Summary of Laboratory Test Results, Phase I & II—Project 422*. Tech Memo 422-47. Center for Transportation Research, University of Texas at Austin, Feb. 1, 1989.
8. *SAS User's Guide: Statistics*. SAS Institute, Inc. Cary, N.C., 1987.
9. V. L. Anderson and R. A. McLean. *Design of Experiments: A Realistic Approach*. Marcel Dekker, Inc., New York, 1974.
10. ACI Committee 209. Prediction of Creep, Shrinkage and Temperature Effects in Concrete Structures. In *Designing for Creep and Shrinkage in Concrete Structures*. ACI Publication SP-76. American Concrete Institute, Detroit, Mich., 1982.
11. J. Lu, H. Castedo, and B. F. McCullough. *Normalization of Models 1 and 2 for Tensile Strength, Modulus of Elasticity, and Drying Shrinkage of Pavement Concrete Made with Texas Coarse Aggregates*. Tech Memo 422-38. Center for Transportation Research, University of Texas at Austin, Feb. 8, 1989.

Publication of this paper sponsored by Committee on Mechanical Properties of Concrete.