

Improving Modulus of Elasticity Prediction in Cement-Based Composites: The Impact of Rubber Particle Incorporation, Nonlinear Regression Optimization, and Hybrid Voigt-Reuss/Reuss-Voigt Models

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Abstract – This study investigates the influence of rubber particles on the stiffness and deformability of cement-based composites, with a particular focus on predicting the modulus of elasticity based on the incorporation rate of rubber particles. Accurate prediction of the modulus of elasticity for these composites presents a challenge due to the tendency of conventional models to either overestimate or underestimate this parameter. The Voigt-Reuss and Reuss-Voigt models, employed as predictive bases, are reliable; however, they exhibit biases in estimating the modulus of elasticity. Nevertheless, these models prove valuable when optimized using nonlinear regression factors derived from polynomial equations of n^{th} order. Despite their tendency to skew results, the Reuss-Voigt and Voigt-Reuss models remain robust tools for predicting the modulus of elasticity of concrete. The optimization process utilizing the calibration factor significantly enhances their predictive accuracy. This research highlights the enhancement of predictive accuracy in models for cement-based composites, thereby contributing to a better understanding and optimal utilization of these materials in structural applications.

Keywords – Stiffness; Deformability; Reuss-Voigt Model; Voigt-Reuss Model; Nonlinear Regression.

I. INTRODUCTION

The elasticity modulus of cement-based materials is an essential characteristic because it greatly influences how concrete deforms when subjected to load, subsequently impacting structural movement [1]. This research seeks to investigate how the incorporation of rubber affects the stiffness and deformability of composite materials. It utilizes the Voigt-Reuss and Reuss-Voigt models for multiphase materials to forecast the modulus of elasticity of cement-based composites based on varying levels of rubber particle integration [2],[3]. Thus, calculating the modulus of elasticity for a unidirectional composite requires deriving expressions for this parameter based on the mechanical and geometric

properties of the material, as well as the volume fractions of the aggregates incorporated into the matrix [4]. Numerous studies have proposed various analytical approaches to estimate the modulus of elasticity of a composite, taking into account the properties of its individual components and their volume fractions [5]. These models, established through basic homogenization techniques, are generally used to idealize the behavior of bi-phased or tri-phased composites [6]. For instance, the Voigt model, which assumes a parallel alignment of material phases, predicts the upper bound for the modulus of elasticity in rubberized concrete [7]. To improve prediction accuracy, De Larrard proposed two hybrid models that integrate both parallel and series distributions: the Voigt-Reuss and Reuss-Voigt models [8]. Additionally, models like those developed by Popovics and Hirsch-Dougill consider the material as a combination of parallel and serial distributions, offering diverse elasticity modulus estimates depending on the phase configurations [9],[10].

Moreover, simplified mathematical frameworks like the Bache and Nepper-Christensen model provide preliminary estimates for the elasticity modulus of rubberized composites [11]. In contrast, more advanced models, such as the Maxwell and Counto models, capture the behavior of materials with either dispersed phases or concentric configurations, providing more accurate predictions of the modulus of elasticity [12],[13]. De Larrard and Le Roy further explored aggregate packing density to enhance modulus predictions in cement-based composites [14]. Distribution-dilution models treat rubber as an isotropic spherical inclusion within an infinite matrix, determining effective mechanical properties through stress-strain relationships derived for microscopically heterogeneous samples [15]. Meanwhile, the Christensen-Lo model estimates the equivalent shear modulus and compressibility by assuming a homogeneous medium that replicates the average stress-strain behavior of a spherical inclusion [16].

Overall, accurately predicting the effective properties of composite materials involves using geometric models that consider macroscopic homogeneity and isotropy [17]. The Voigt-Reuss and Reuss-Voigt models [8], in particular, are fundamental for defining the theoretical upper and lower bounds of the modulus of elasticity in composite materials, making them crucial tools for evaluating and optimizing multiphase systems.

This study offers a comprehensive evaluation of the hybrid Voigt-Reuss and Reuss-Voigt models for predicting the modulus of elasticity in cementitious composites, with a specific focus on how rubber particles influence stiffness and deformability rates. By integrating analytical models that account for the material properties and volume fractions of composite constituents, this research provides deeper insights into the complex mechanical behavior of rubberized concrete under various loading conditions.

The findings of this work have a significant impact on civil engineering applications. Understanding the modulus of elasticity for cement-based materials is essential for designing structures that can withstand external loads while maintaining structural integrity. Accurate predictions of the modulus of elasticity in rubberized concrete enable engineers to optimize the design of infrastructure elements such as bridges, pavements, and buildings, enhancing their durability and resilience. Furthermore, utilizing rubberized concrete contributes to sustainable construction practices by recycling rubber waste and reducing environmental impact. Overall, this study enriches the field of civil engineering by advancing knowledge on the mechanical performance of innovative composite materials and their practical applications in infrastructure development.

II. MATERIALS AND METHOD

A. *Materials*

This research applies traditional cement concrete formulation techniques, typically used for pavement design, to rubberized composite concretes. The Dreux-Gorisse method [18] was employed, as it minimizes cement content and maximizes aggregate use, resulting in enhanced mechanical properties for rubberized concrete. To ensure a valid comparison with conventional concrete and mitigate the adverse

effects of excessive water on mechanical strength, a constant water-to-cement (w/c) ratio of 0.45 was maintained throughout all mixes. The study evaluated the performance impact of incorporating rubber waste by preparing two concrete variants—Crumb Rubber Concrete (CRC) and Ground Tire Rubber Concrete (GTRC)—with varying substitution levels of sand by rubber particles (0, 10, 15, 20, and 25% by volume). The detailed formulation and methodology are outlined in a previous publication [19].

Dry ingredients were initially blended in a motorized planetary mixer. Subsequently, water and a fixed amount of superplasticizer (SP) were introduced, and the mixture was blended for three minutes until achieving a homogeneous consistency. An air-entraining agent (AEA) was then added, followed by an additional two minutes of mixing. The concrete was poured into molds in three successive layers, each compacted on a vibrating table for one minute to ensure proper consolidation. After 24 hours, the specimens were demolded and transferred to a curing chamber, where they were kept for 28 days under standardized conditions ($20 \pm 2 \text{ }^\circ\text{C}$ and 60-80% relative humidity).

B. Method

To achieve a more precise estimation of the elastic modulus in composite materials, De Larrard introduced two hybrid models that integrate both parallel and series distributions: the Voigt-Reuss model and the Reuss-Voigt model [2], [3]. The Voigt-Reuss model, referred to as the (combined VR) model and depicted in Fig. 1, is expressed through the equation provided below [2], [3].

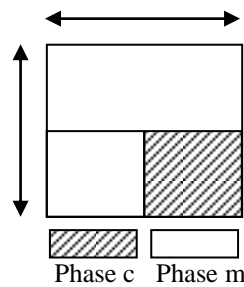


Fig. 1 Illustration of the Voigt-Reuss Composite Model

$$E_{c_VR} = \frac{(E_m \beta)}{\gamma} \tag{1}$$

Where the empirical factors β and γ represent the combined system of this model and are defined by the equations presented below:

$$\begin{cases} \beta = (E_m) + (V_r^{2/3}) \times (E_r - E_m) \\ \gamma = \beta(1 - V_r^{1/3}) + (E_m V_r^{1/3}) \end{cases} \tag{2}$$

The Reuss-Voigt model (combined RV), as illustrated in Fig. 2, is also calculated using the expression provided in the equation shown below [2], [3]:

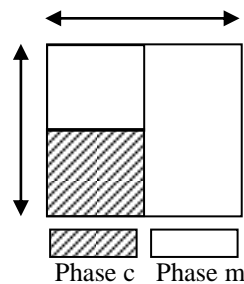


Fig. 2 Illustration of the Reuss-Voigt Composite Model

$$E_{c_RV} = E_m + V_r^{1/3}(\xi - E_m) \tag{3}$$

Where the empirical factors θ and ξ represent the combined system of this model and are given as follows:

$$\begin{cases} \theta = E_r + V_r^{2/3}(E_m - E_r) \\ \xi = \frac{E_m E_r}{\theta} \end{cases} \tag{4}$$

III. RESULTS

The results obtained from the biphasic modeling of the studied composites are summarized in Table 1 and compared with the experimental results. The findings indicate an increasing discrepancy between the two sets of results as the rubber particle incorporation rate in the mixtures rises. Furthermore, Fig. 3 illustrates the correlation among the various values, revealing that the theoretical results are biased compared to the experimental data, with a moderately close concordance. Although the theoretical values remain in proximity to the experimental data, the observed discrepancy can be attributed to the assumption that concrete is treated as a homogeneous and isotropic material in these models. It is important to note that these models differ in their hybrid considerations of parallel and series configurations, which may lead to a misalignment in estimation relative to experimental findings.

Table 1. Numerical values of Voigt-Reuss and Reuss-Voigt models and variation of the relative errors calculated in relation to the experimental results

Mix	β	γ	θ	ξ	Δ_{VR} (%)	Δ_{RV} (%)
CC0	36.49	36.49	0.022	36.49	0.00	0.00
CRC10	31.64	33.41	4.86743559	0.16492874	17.87	20.70
CRC15	30.14	32.79	6.36763825	0.12607186	35.95	13.58
CRC20	28.83	32.34	7.67785607	0.10455783	51.44	7.73
CRC25	27.72	32.02	8.79189945	0.09130905	70.20	0.43
GTRC10	31.11	33.17	5.39987075	0.14866652	5.13	30.78
GTRC15	29.41	32.53	7.09332771	0.11317396	13.09	29.85
GTRC20	27.95	32.08	8.55569054	0.09382995	27.00	24.60
GTRC25	26.72	31.77	9.78720439	0.08202342	42.15	18.25

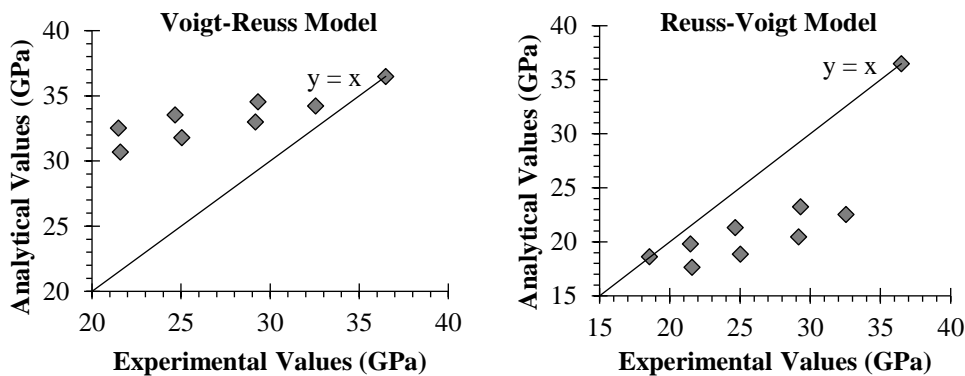


Fig. 3 Correlation between theoretical values and experimental values according to Voigt-Reuss and Reuss-Voigt models

To fit a model to the data provided and estimate the corresponding coefficients, non-linear regression can be used.

A script using the Matlab calculation code fits a linear model to the data using non-linear regression. The function to be fitted is of the polynomial form:

$$P(x) = \sum_{i=0}^8 a_i x^i \tag{5}$$

Where:

$P(x)$ is the polynomial.

a_i represents the coefficients of the polynomial, where i varies from 0 to 8.

x is the variable of the polynomial.

After checking and comparing the model with the data, the optimal parameters are estimated and displayed at the Table 2, with:

Table 2. Coefficients and Statistical Parameters for Polynomial Regression Models (VR and RV)

Model	VR	RV
a_8	1.69	0.04
a_7	-447.6638	-6.4
a_6	52007.7482	498.05
a_5	-3451274.99	-21968.58
a_4	143088759	601484.54
a_3	-3795306019	-10475137.66
a_2	62893296416	113387378.7
a_1	-5.95334×10^{11}	-697803345.1
a_0	2.46453×10^{12}	1870068009
Standard Error	0.0009	0.001
R	1	1
R ²	1	1

The results obtained are presented in Fig. 4 and indicate that the values predicted by the model closely align with the observed values. This is supported by several observations, including the fact that the standard errors are very low, approximately 0.0009 for VR and 0.001 for RV, respectively, with a standard deviation of 0.003 for both groups. This suggests that the observed values are very close to the values predicted by the model. In other words, the dispersion of the observed values around the predicted values is minimal, with an average relative error of 0.0169% for VR and 0.0205% for RV. The calculation of these errors was performed according to the equations presented below:

$$Standard.Error = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n - p}} \tag{6}$$

Where n is the number of observations, p is the number of parameters estimated in the model, y_i represents the observed values, and \hat{y}_i represents the predicted values.

$$Relative.Error = Standard.Error / \bar{y} \tag{7}$$

Where \bar{y} is the mean of the observed errors.

The correlation coefficient R and the coefficient of determination R^2 are both equal to 1, indicating a perfect correlation between the observed and predicted values. This implies that the fitted model perfectly explains the variation in the observed data. The calculation of the correlation coefficient was performed according to the equation presented below:

$$R = \frac{\sum_{i=1}^n (y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})}{\sqrt{\sum_{i=1}^n (y_i - \bar{y})^2} \sqrt{\sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})^2}} \quad (8)$$

Where \bar{y} is the mean of the observed values and $\bar{\hat{y}}$ is the mean of the predicted values.

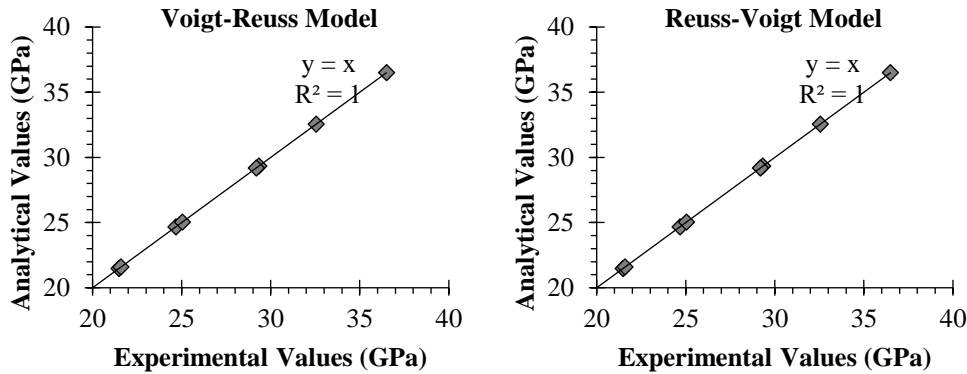


Fig. 4 Correlation between theoretical values and experimental values according to Voigt-Reuss and Reuss-Voigt models After optimization

In conclusion, the observed results are in very good agreement with the values predicted by the models, indicating that the models is highly reliable for predicting the values of the elasticity modulus in this context.

IV. DISCUSSION

The implementation of this modeling leads to an additional observation regarding the behavior of the elastic modulus in relation to the rubber content within the composites. Specifically, the model provides an approximate depiction of how the elastic modulus varies with the amount of rubber incorporated. However, this assertion holds true primarily for smaller inclusion dosages, prompting a deeper investigation into the factors that contribute to less accurate descriptions, particularly in the case of Crumb Rubber Concrete (CRC) mixtures.

This discrepancy can be attributed to the models' assumption that the material is perfectly homogeneous, characterized by a uniform transverse thickness without any interfacial defects between the rubber and the cement matrix. In reality, as illustrated in Fig. 5, the rubber particles employed exhibit varying shapes and thicknesses, leading to a random distribution and moderately homogeneous dispersion within the cement matrix. This results in the formation of defects, creating interfacial transition zones (ITZ).

Furthermore, the inherent lower apparent density of elastomers compared to mineral aggregates may contribute to segregation phenomena, which tend to create additional voids within the mixtures based on their size and volume of incorporation into the cement matrix. This factor elucidates the observed differences and variations in rigidity, toughness, and energy dissipation between the two concrete groups. Consequently, mixtures incorporating smaller-sized inclusions emerge as the most suitable composites for the design of various structures, such as rigid pavements.

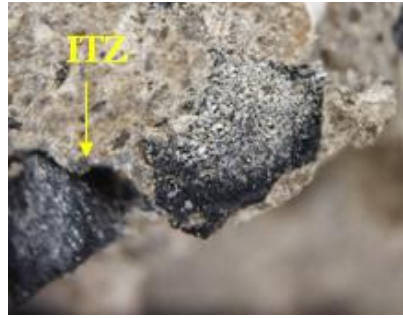


Fig .5 Optical micrograph showing the interfacial transition zone (ITZ) between the cement matrix and rubber particle

V. CONCLUSION

The calculated values of the elastic modulus using the Voigt-Reuss and Reuss-Voigt analytical models exhibit slight biases but remain in close proximity to the experimental data. However, the relative variation estimated between the theoretical and experimental measurements can be more pronounced for Crumb Rubber Concrete (CRC) mixtures. These findings indicate that these models serve as powerful predictive tools when properly optimized, while also highlighting an issue related to the interfacial transition zone (ITZ) between the rubber particles and the cement matrix. The challenge of achieving a homogeneous and continuous bond arises from the geometric discrepancies in shape and thickness, as well as the inherent heterogeneity of the materials within the concrete. This leads to variations in the toughness of rubberized composites, thereby suggesting that Ground Tire Rubber (GTR) inclusions are the most advantageous for incorporation into the cement matrix.

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