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Modeling Hyperelastic Behavior of Natural Rubber/Organomodified Kaolin Composites Oleochemically Derived from Tea Seed Oils (*Camellia sinensis*) for Automobile Tire Side Walls Application

Chukwutoo Christopher Ihueze¹ and Chinedum Ogonna Mgbemena^{2*}

¹Department of Industrial Production Engineering, Nnamdi Azikiwe University, Awka, Nigeria.

²Department of Mechanical Engineering, Federal University of Petroleum Resources, Effurun, Nigeria.

Authors' contributions

This work was carried out in collaboration between the both authors. Author CCI designed the study, wrote the draft of the article. Author COM managed the experimental process, FEA and took care of formatting and provided finishing touch to this manuscript. Both the authors read and approved the final manuscript together.

Original Research Article

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ABSTRACT

This paper is on the modeling and prediction of limit stresses of Natural Rubber/Organomodified kaolin composites oleochemically derived from Tea Seed Oils (*Camellia sinensis*). The stress-strain data reports of Natural Rubber/Tea Seed Oil modified (NR/TSO) kaolin were used to develop hyperelastic models using ANSYS 14.0 work bench. Arruda-Boyce, Mooney-Rivlin 9 Parameter, Polynomial 3rd Order and Yeoh 3rd Order models were found to give perfect fit for NR/TSO modified kaolin composites. The energy absorption capabilities were measured on the functions derived from stress-strain data to establish the toughness of Natural Rubber/Unmodified Kaolin (NR/UMK) and NR/TSO modified Kaolin. The NR/UMK has its approximate strain energy as 29.12MJ/m³ at 2 parts per hundred rubber (phr) while the NR/TSO kaolin composite has its approximate strain energy as 31.12MJ/m³. The orthogonal stresses, the principal stresses and yield stresses are found to be lower than the ultimate tensile strength of

*Corresponding author: E-mail: mgbemena.ogonna@fupre.edu.ng;

0.7875MPa hence the material is safe within load range of its ultimate strength. Plane stress analysis with ANSYS APDL 14.0 gave limit stresses distribution in terms of von-Mises stresses in the range 0.781869MPa-0.792847MPa. The maximum principal stress is found to be higher than the ultimate tensile strength of 0.7875MPa hence the material is safely specified with load range of von Mises, 0.781869MPa-0.7875MPa. Finally it was observed that organomodification of kaolin with tea seed oil (TSO) increases the strength of Natural Rubber composites.

Keywords: Hyperelastic behavior; energy absorption; strain energy; von-mises stresses; plane stress.

1. INTRODUCTION

Usually design engineers are in search of materials that will be robust in service that selection of materials of design is of great concern for service delivery. In an isotropic material subjected to uniaxial stress, failure prediction is simply to ensure that applied uniaxial stress does not exceed the ultimate strength which is usually specified in material data sheet but most of the times serving materials are subjected to multi-axial stress state that different and more robust techniques are needed to predict failure. This is to say that if the orthogonal stresses σ_x , σ_y are involved; failure prediction is not simply a question of ensuring that the orthogonal stresses does not exceed the material ultimate strength because at values of orthogonal stresses σ_x , σ_y below the materials ultimate strength there can be plane within the material where the stress reaches the ultimate strength and this will initiate failure. Crawford [1] reported the various failure theories on maximum stress criterion, maximum strain criterion and Tsai-Hill criterion as appropriate for predicting failure of composite materials. Ihueze et al. [2] applied Distortion Energy Theory (DET) implemented with ANSYS software to predict failure of plantain composites subjected to multi-axial stress state.

Previous studies show that prediction of the onset of failure is more important than the knowledge of the ultimate strength of material [1-5]. Hence by trying to predict yield of material that requires the knowledge of the associated orthogonal stresses, principal stresses and shear stresses of the multi-axial stressed material as evidenced in von Mises stress theory, a robust technique like the finite element model is needed to solve a material model that captures the material properties and external effects.

Natural Rubber composites have numerous industrial application areas such as automobiles, aerospace, industrial machinery and packaging. In automobiles, natural rubber composites are applied in vehicle tire sidewalls and tubes, as door seals and engine seals. In aerospace, they are used in fuel systems. In other engineering fields, they have been applied in conveyor belts, meteorological balloons and bearings of foundations.

Several researchers have developed a theoretical stress-strain relation that fits experimental results for hyperelastic materials [6-12]. Mooney proposed a phenomenological model with two parameters based on the assumptions of a linear relation between the stress and strain during simple shear deformation [13]. Treloar published the neo-Hookean material model which is based on the statistical theory with only one material parameter. The neo-Hookean model developed by Treloar was proved to be a special case of the Mooney model [14]. The Mooney and neo-Hookean strain energy function have played an important role in the development of the nonlinear hyperelastic theory and its applications [15-16].

Rivlin [17-19] modified the Mooney model to obtain a general expression of the strain energy function expressed in terms of strain invariants. Yeoh [20] developed one of the most successful hyperelastic models in the form of a third-order polynomial of the first invariant of the right Cauchy–Green tensor. A high-order polynomial model with the form of a natural logarithm of the first invariant has been proposed by Gent. In 1972, Ogden proposed a strain energy function expressed in terms of principal stretches, which is a very general tool for describing hyperelastic material. An excellent agreement has been obtained between Ogden's formula and Treloar's experimental data for extensions of unfilled natural rubber up to 700% [21-22]. However, the parameter identification is complicated because of the purely phenomenological character of the Ogden strain energy function.

In this study, we will employ the experimental results of Mgbemena [23] to investigate on the hyperelasticity of Natural Rubber composites; model and analyze the stress strain response using ANSYS Workbench 14.0; model hyperelasticity and predict failure, establishing distribution of maximum principal stresses and the von Mises stress distribution which gives the critical stresses of various locations of the material.

2. METHODOLOGY

2.1 Materials and Data

The Tea seed oil modified kaolin used in this study was prepared according to the methods published by the following authors [24-26].

2.1.1 Preparation of rubber vulcanizates

A series of Tea seed oil modified kaolin/natural rubber composites were prepared by melt blending as explained in the recipes of Table 1. Melt blending involves dispersal and exfoliation of an organoclay into an elastomer whilst it is being softened by application of high-shear forces from a two-roll mill. NR were initially laminated for 5-10 min in the open two-roll mill around 30–40°C. Thereafter, the rubbers were blended with accelerants, activators, kaolin, softeners and lastly, Sulphur was added. The mixtures were plasticized for about 12–15 min and thin-passed several times at 90°C. The obtained Natural Rubber/Kaolin compounds were allowed to cure. Rubber vulcanizates sheets of dimension 90 mm × 90 mm × 1.5 mm were prepared by compression molding of the mixes at 140°C for 10 min on an electrically heated, semi-automatic hydraulic press (MODEL INDUDYOG DS-SD-HMP/25) at 400 Pa and curing takes place at the same temperature and pressure.

Table 1. Recipes of the rubber compounds

Ingredients (phr)	UMK	TSOMK
Natural Rubber	100	100
Zinc Oxide	5	5
Stearic Acid	2	2
URK	2,6,10	-
MRK	-	2,6,10
MBT	2	2
Sulphur	2	2

UMK is the unmodified Kaolin; TSOMK is the TSO-modified Kaolin; MBT is MercaptoBenzothiazole

The materials and data of this work are based on the uniaxial tests results of replicated samples of natural rubber/unmodified kaolin composites (NR/UMK and natural rubber tea seed oil modified kaolin (NR/TsOMK) as reported in [23] and exhibited in Figs. 1 and 2.

2.2 Hyperelastic Modeling and Curve Fitting of Stress-Strain Data

Hyperelastic models are generally employed in most Finite Element Analysis (FEA) software. The stress-strain data is required for the FEA of rubber materials. The material parameters of the various composites optimized in this work were determined by the fitting of the strain energy function to stress-strain data using ANSYS Workbench 14.0. The optimization process is used in the ANSYS software to minimize the error with respect to the model's parameter. The uniaxial test data was used to obtain the coefficients of the strain energy function and the hyperelastic models are obtained to provide a good fit between the predictions from the model and stress- strain data.

2.3 Estimation of Energy Absorption Capabilities of the Composites

The energy absorption capabilities of the optimum setting of the composites can be estimated using trapezoidal rule to compute the area under the stress strain function's curve. Newton-Cotes integration formulas (trapezoidal rule, Simpson's rule and Richardson's extrapolation (Romberg integration)) are possible integration schemes to evaluate the area under the curve.

2.4 Failure Analysis

The best estimation method for predicting the onset of yielding, for materials exhibiting equal strengths in tension and compression is the octahedral shear stress theory (distortion energy or Henky-von Mises) which is classically expressed as [27]:

$$\tau_0 = \frac{1}{3} [(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]^{1/2} \quad (1)$$

This can be expressed in terms of orthogonal component stresses as

$$\tau_0 = \frac{1}{3} [(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)]^{1/2} \quad (2)$$

However the limiting value of the octahedral shear stress is that which occurs during uniaxial tension at the onset of yield. This limiting value is

$$\tau_0 = \frac{\sqrt{2}S_y}{3} \quad (3)$$

By expressing this in terms of the principal stresses and a design factor, we have

$$\frac{S_y}{n} = \frac{3}{\sqrt{2}} [\tau_0]_{\text{lim}} = \frac{1}{\sqrt{2}} [(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]^{1/2} = \sigma' \quad (4)$$

The term σ' is called the von Mises stress. It is the uniaxial tensile stress that induces the same octahedral shear (or distortion energy) in the uniaxial tension test as does the triaxial stress state in the actual part.

Where,

$\sigma_1, \sigma_2, \sigma_3$ = are the ordered principal stresses,

$\sigma_x, \sigma_y, \sigma_z$ = are the orthogonal stresses in x, y and z-directions respectively,

$\tau_{xy}, \tau_{yz}, \tau_{zx}$ = orthogonal shear stresses,

S_y = uniaxial yield stress,

σ' = von Mises stress,

n = design safety factor.

The plane stress materialmodel usually implemented in most FE solvers for linear elastic isotropic materials for failure analysis is expressed as:

$$\begin{bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{bmatrix} = \frac{E}{1-\mu^2} \begin{bmatrix} 1 & \mu & 0 \\ \mu & 1 & 0 \\ 0 & 0 & (1-\mu)/2 \end{bmatrix} \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{bmatrix} \quad (5)$$

This means that with the material properties of elastic modulus E and Poisson's ratio μ the orthogonal stresses and principal stresses can be estimated in a finite element solver system. Also implemented is the strain-displacement relationships expressed as:

$$\varepsilon_x = \frac{\partial u}{\partial x}, \varepsilon_y = \frac{\partial v}{\partial y}, \gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \quad (6)$$

The beauty of this analysis includes the evaluation of yield stresses obtained as von Mises stresses, orthogonal stresses and etc. In this work ANSYS APDL 14.0 was used to solve for plane stresses and subsequently the yield stress distribution.

3. RESULTS AND DISCUSSIONS

Figs. 1 and 2 presents the uniaxial tests results of unmodified and tea seed oil modified Natural Rubber composites. Both figures show hyperelastic nature of Rubber composites as the recorded maximum strain at failures exceeded 500%.

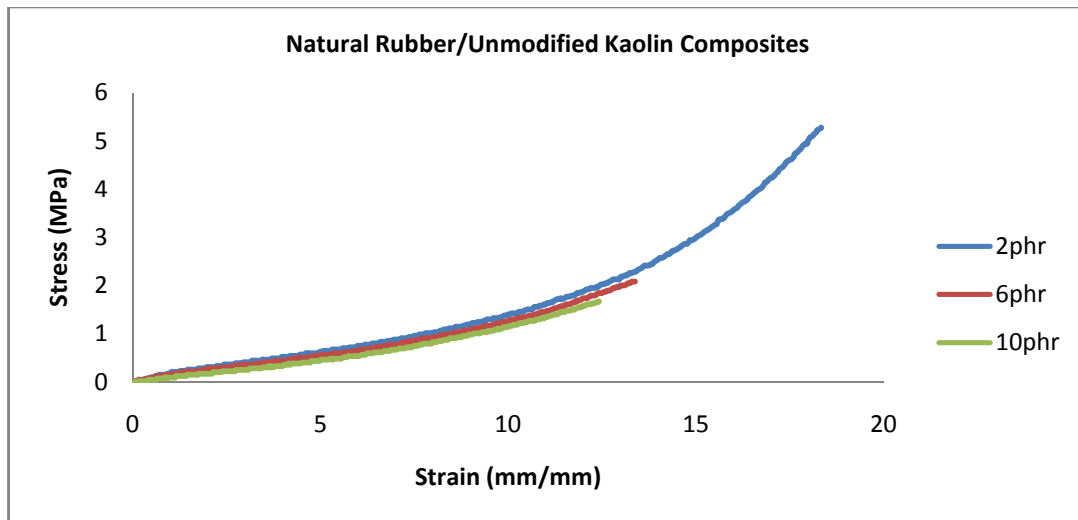


Fig. 1. Natural rubber/unmodified kaolin composites

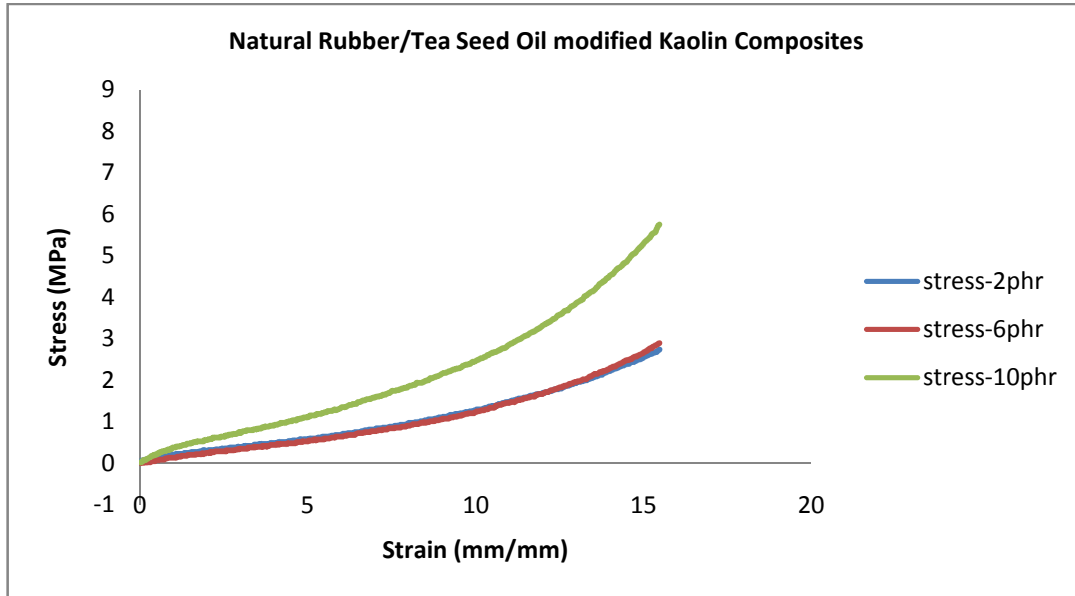


Fig. 2. Natural rubber/tea seed oil modified kaolin composites

Figs. 3, 4 and 5 are finite element models representing NR/TSO modified kaolin composites obtained by inputting the stress-strain data of NR/TSO modified kaolin composites of Fig. 2 for 10phr (parts per hundred rubber) in ANSYS 14.0 workbench. Tables 2, 3 and 4 gives the ANSYS 14.0 results of material constants or parameters for Arruda Boyce model, Mooney-Rivlin Parameter model and the Yeoh 3rd order model respectively. The actual models are established by using the values of Table 2-4 in the relevant equations of the material models.

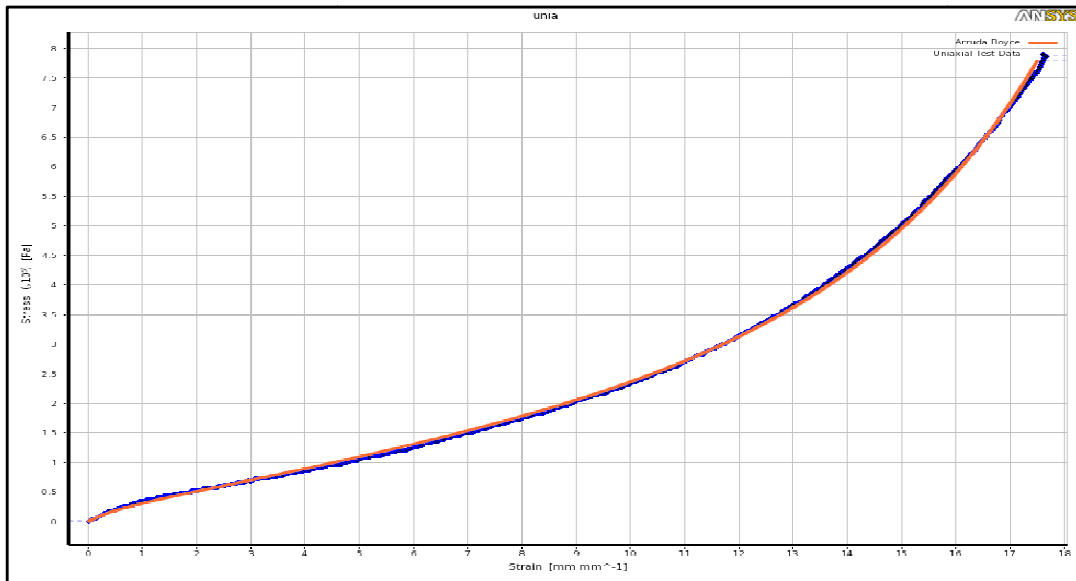


Fig. 3. Arruda-Boyce model for NR/TSO modified kaolin at 10phr

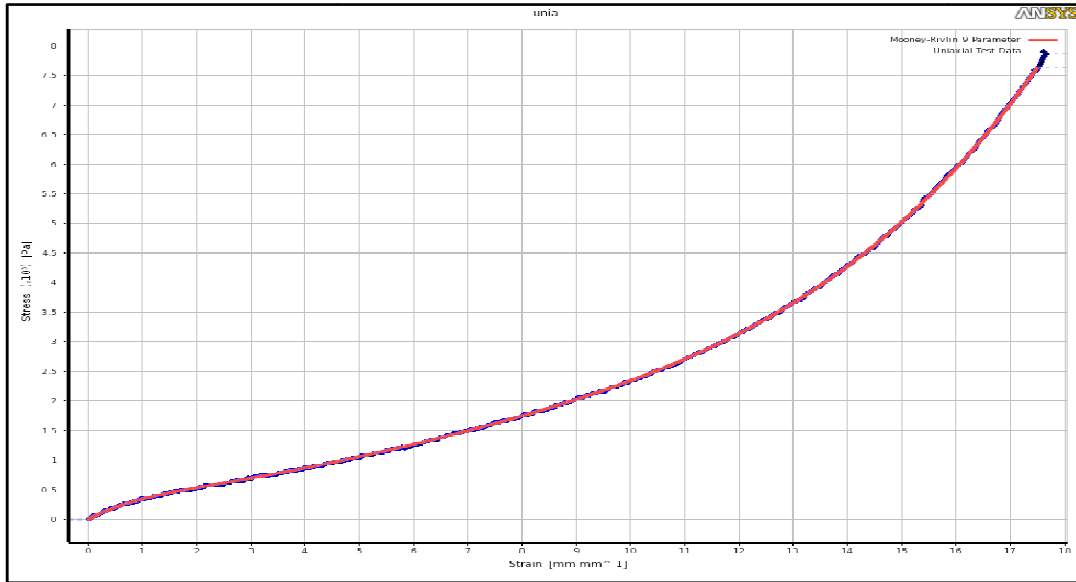


Fig. 4. Mooney Rivlin 9 parameter model for NR/TSO modified kaolin at 10phr

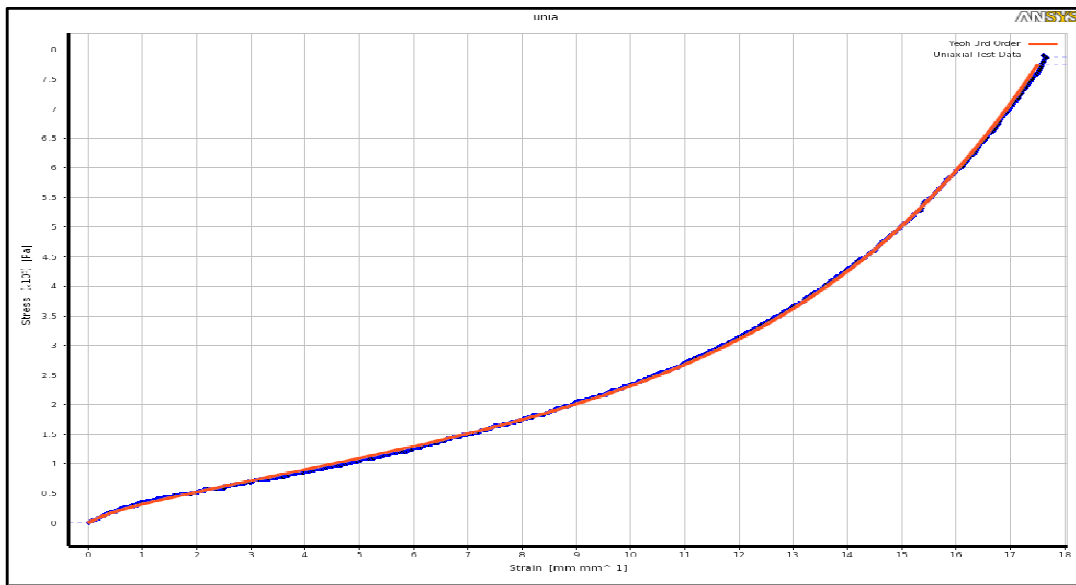


Fig. 5. Yeoh 3rd order model for NR/TSO modified kaolin at 10phr

Table 2. Computed parameters for Arruda-Boyce

Coefficient name	Calculated value
Incompressibility Parameter D1	0
Initial Shear Modulus μ	17430Pa
Limiting network stretch	-11.903
Residual	1.3245

Table 3. Computed parameters for Mooney-Rivlin nine parameter model for NR/TSO modified kaolin at 10phr (parts per hundred rubber)

Coefficient name	Calculated value
Incompressibility Parameter D1	0Pa ⁻¹
Material parameter C01	-4300.5Pa
Material parameter C02	-1.288E+05Pa
Material parameter C03	-16873Pa
Material parameter C10	12807Pa
Material parameter C11	2.4392E+05Pa
Material parameter C12	29191Pa
Material parameter C20	-1.1691E+05Pa
Material parameter C21	2.5878Pa
Material parameter C30	-0.0381Pa
Residual	0.26642

Table 4. Computed parameters for Yeoh 3rd order parameter model for NR/TSO modified kaolin at 10phr

Coefficient name	Calculated value
Incompressibility Parameter D1	0Pa ⁻¹
Incompressibility Parameter D2	0Pa ⁻¹
Incompressibility Parameter D3	0Pa ⁻¹
Material parameter C10	9048.7Pa
Material parameter C20	0.30743Pa
Material parameter C30	0.033796Pa
Residual	0.88043

The trapezoidal rule for unequal segments (varying step size) is expressed in [28] as:

$$I = h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \dots + h_n \frac{f(x_{n-1}) + f(x_n)}{2} \quad (7)$$

Data of Figs. 1 and 2 were used to generate data for Tables 5 and 6 respectively and applied to equation (7) to implement trapezoidal rule for evaluation of energy absorbed.

Table 5. Data for application of trapezoidal rule to unequal segments of function (f(x)) of NR/unmodified kaolin composites at 2phr

I	x	H	F(x _i)	N	$h_n \frac{f(x_{n-1}) + f(x_n)}{2}$
0	0.02		0.01		
1	0.54	0.52	0.10	1	0.0286
2	2.06	1.52	0.31	2	0.3116
3	2.88	0.82	0.39	3	0.2870
4	3.90	1.02	0.49	4	0.4488
5	5.54	1.64	0.68	5	0.9594
6	6.26	0.72	0.78	6	0.5256
7	7.78	1.52	1.10	7	1.4288
8	8.54	0.76	1.12	8	0.8512
9	9.68	1.14	1.33	9	1.3965

Table 5 continued.....

10	10.82	1.14	1.58	10	1.6587
11	12.24	1.42	1.95	11	2.5063
12	13.44	1.20	2.32	12	2.5620
13	14.58	1.14	2.80	13	2.9184
14	15.68	1.10	3.38	14	3.3990
15	16.60	0.92	3.95	15	3.3718
16	18.02	1.42	5.05	16	6.4610
I=Total					29.1147

The area under the stress strain curve response of NR/unmodified composite is then estimated as 29.12MJ/m³.

Table 6. Data for application of trapezoidal rule to unequal segments of function (f(x)) of NR/TSO kaolin composites at 10phr

I	x	h	F(x _i)	N	$h_n \frac{f(x_{n-1}) + f(x_n)}{2}$
0	0.04		0.02		
1	1.22	1.18	0.41	1	0.2537
2	1.60	0.38	0.50	2	0.1729
3	2.74	1.14	0.69	3	0.6783
4	4.24	1.50	0.97	4	1.245
5	5.40	1.16	1.18	5	1.247
6	6.70	1.3	1.51	6	1.7485
7	7.58	0.88	1.74	7	2.86
8	8.34	0.76	1.93	8	1.3946
9	9.74	1.40	2.37	9	3.01
10	10.54	0.80	2.66	10	2.012
11	12.08	1.54	3.35	11	4.6277
12	13.00	0.92	3.86	12	3.3166
13	14.14	1.14	4.61	13	4.8279
14	14.90	0.76	5.20	14	3.7278
I=TOTAL					31.122

The area under the stress strain curve response of NR/unmodified composite is then estimated as 31.12MJ/m³.

Figs. 6-11 presents the elastic stresses associated with the application of NR/TSO modified kaolin evaluated with ANSYS APDL 14.0 using experimentally derived elastic constants (elastic modulus and Poisson’s ratio), material density and assumption of linear elastic-isotropic material model to implement the plane stress. von Mises stresses were evaluated to be in the range 0.781869MPa-0.792847MPa while the shear stresses are within the range 0.07591-0.07597MPa and the orthogonal stresses in x and y are -0.0037951386MPa-0.01186MPa and 0.7875MPa respectively as depicted in Figs. 6 and 7.

Fig. 9 shows that at 2phr the unmodified kaolin natural rubber composite is more hyperelastic. This may be due to the enhancement of cure reaction by intercalated silicate galleries of the unmodified kaolin at low volume fractions. While Fig. 10 shows that TSO modified kaolin rubber composite is more hyperelastic at 10phr which may be attributed to the overall increase in the ultimate state of cure and possible co-crosslinking of the

unsaturation sites of TSO with those of NR during vulcanization and to the alkaline nature of TSO modified kaolin [26,29].

Figs. 12-14 compares stresses distribution of Natural Rubber unmodified kaolin composites at 10phr with Natural Rubber TSO modified kaolin composites to establish that the modification of kaolin increases the strength of natural rubber. The von-Mises stresses values of Fig. 11 of NR/TSO kaolin are higher than that of NR/unmodified kaolin of Fig. 14.

The situation where the applied orthogonal and principal stresses are higher than the ultimate strength of material is unacceptable, so that design engineer must apply load based on von Mises stresses not exceeding the ultimate strength of material. This situation is pronounced in Figs. 9 and 11 where the values of the applied local stresses are more than the ultimate strength of material with value 0.7875MPa.

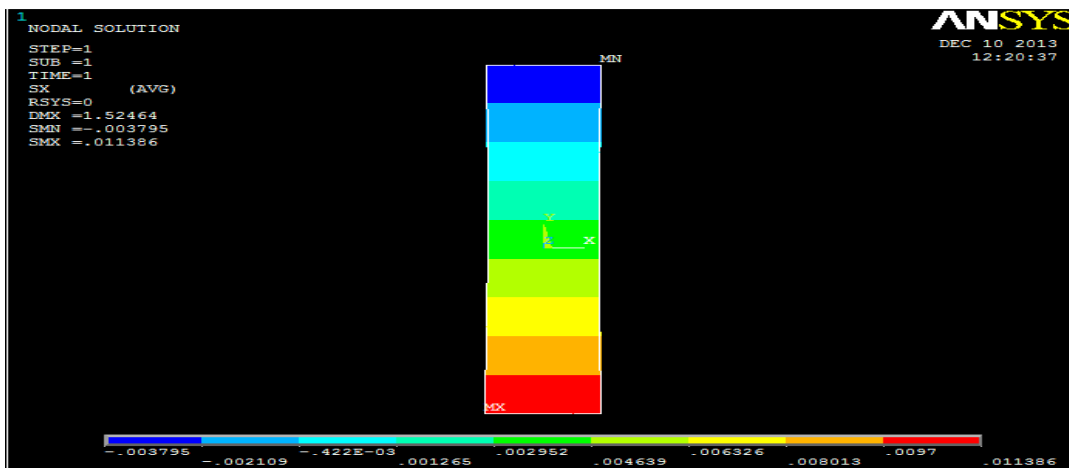


Fig. 6. ANSYS APDL 14.0 Contour plot of distribution of X component orthogonal stresses for NR/TSO kaolin at 10phr

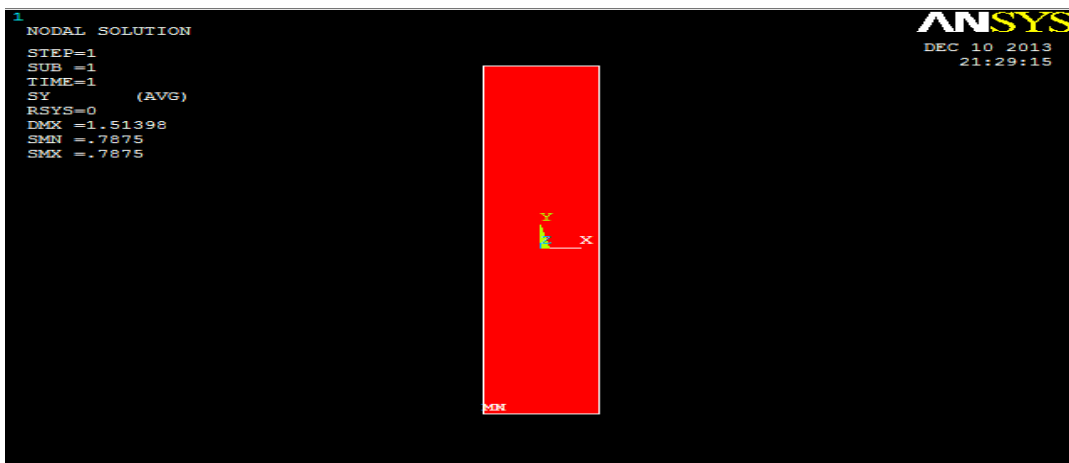


Fig. 7. ANSYS APDL 14.0 Contour plot of distribution of Y component orthogonal stresses for NR/TSO kaolin at 10phr

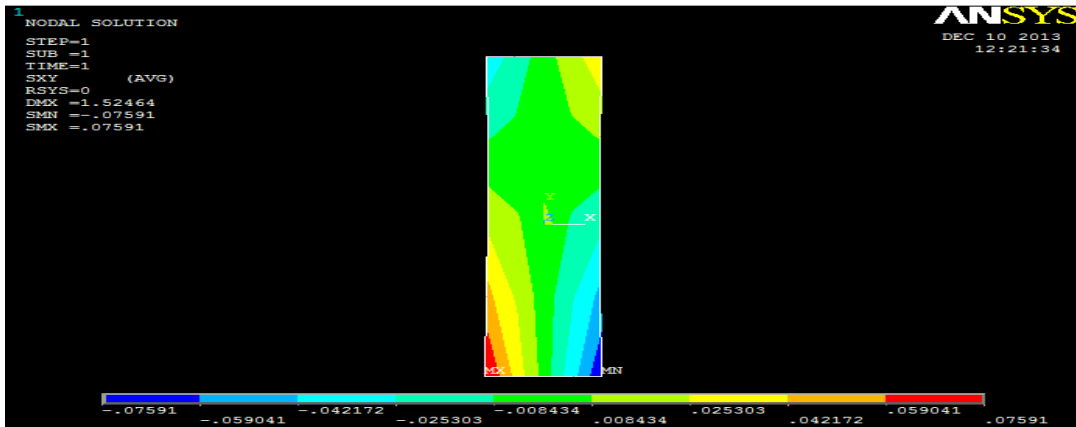


Fig. 8. ANSYS APDL 14.0 Contour plot of distribution of XY shear stress for NR/ TSO kaolin at 10phr

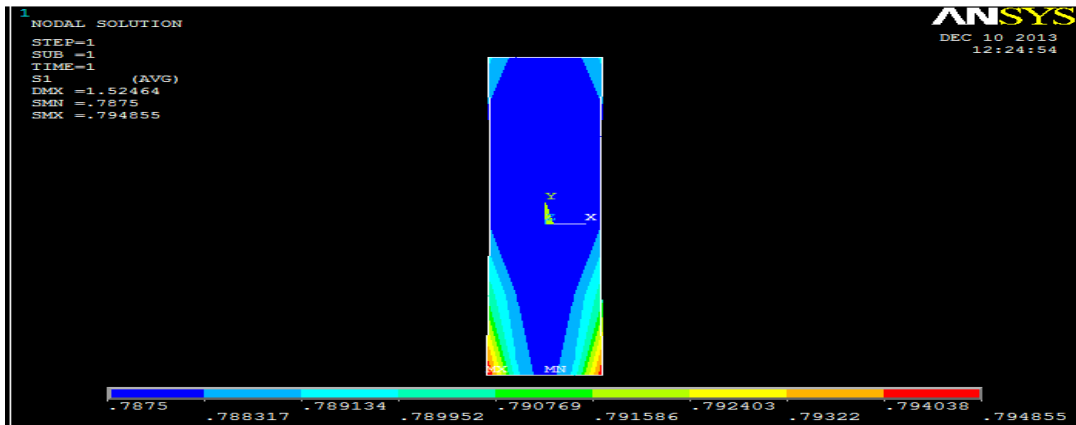


Fig. 9. ANSYS APDL 14.0 Contour plot of distribution of maximum principal stress for NR/TSO kaolin at 10phr

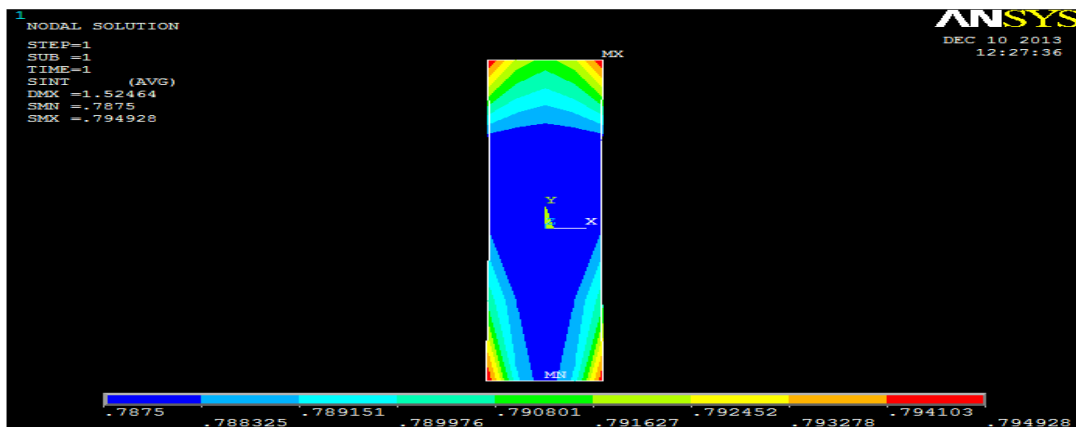


Fig. 10. ANSYS APDL 14.0 Contour plot of distribution of stress intensity for NR/ TSO kaolin at 10phr

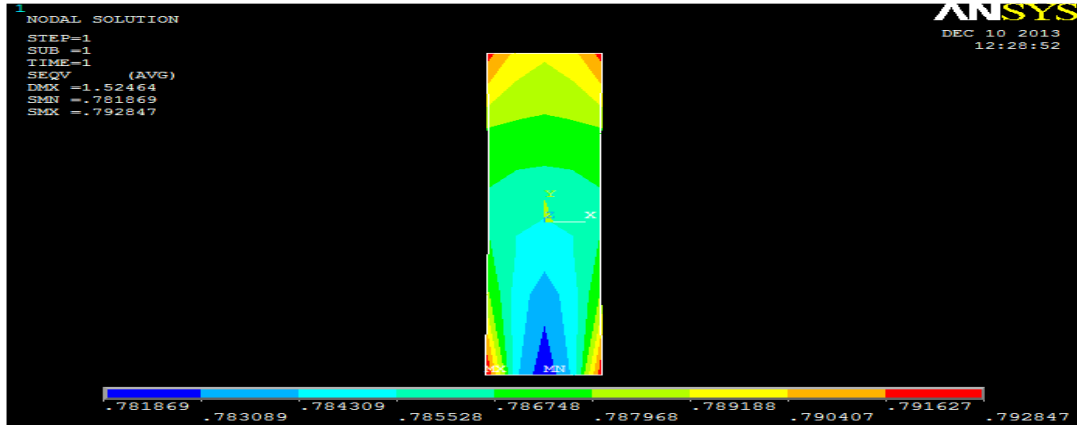


Fig. 11. ANSYS APDL 14.0 Contour plot of distribution of von Mises stress for NR/ TSO kaolin at 10phr

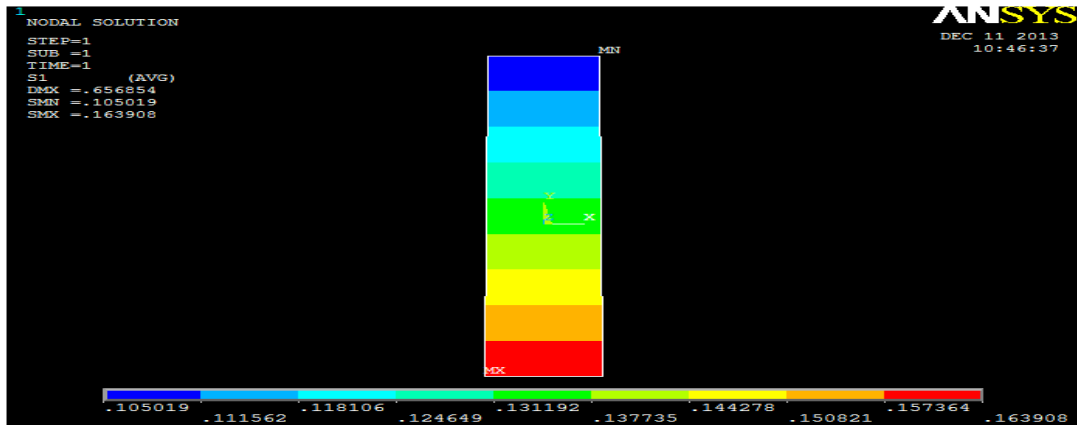


Fig. 12. ANSYS APDL 14.0 Contour plot of distribution of maximum principal stresses for NR/unmodified kaolin at 10phr

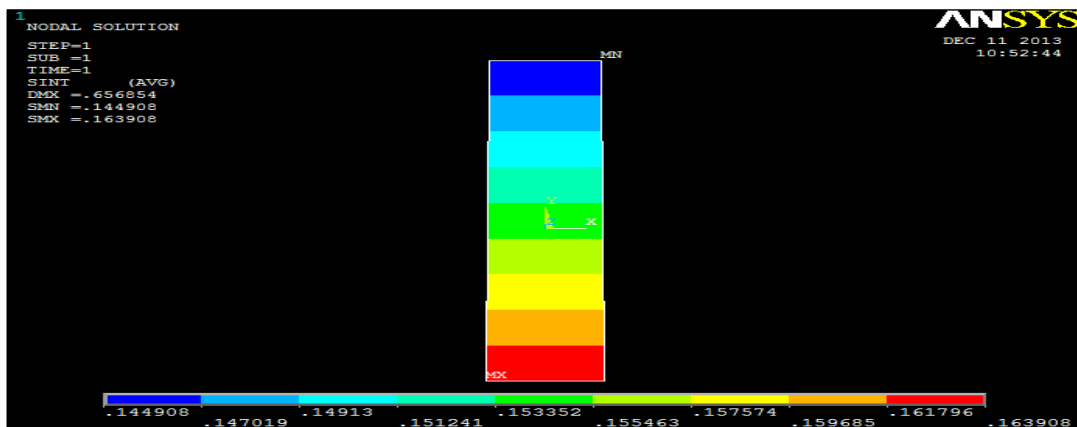


Fig. 13. ANSYS APDL 14.0 Contour plot of distribution of stress intensity for NR/unmodified kaolin at 10phr

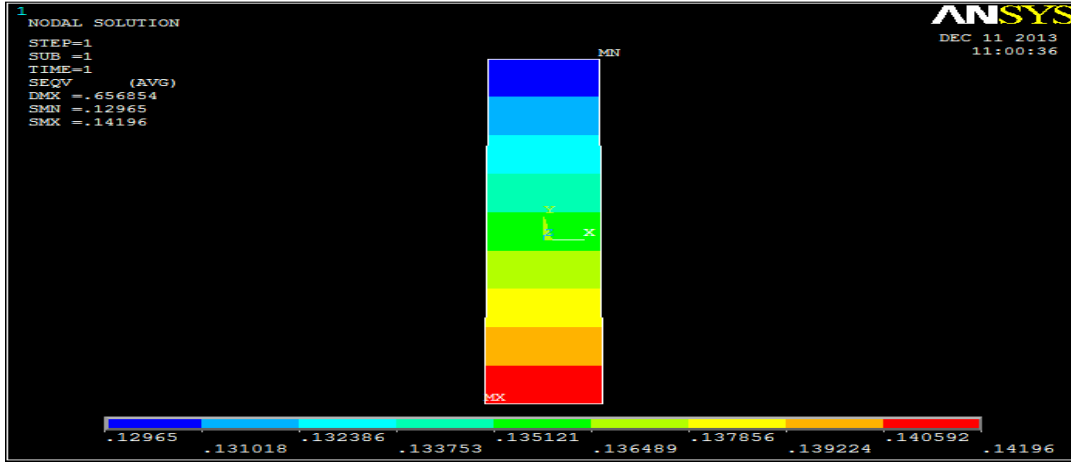


Fig. 14. ANSYS APDL 14.0 Contour plot of distribution of von Mises stress for NR/unmodified kaolin at 10phr

Table 7 gives comprehensive results of the stresses associated with plane stress analysis with ANSYS APDL 14.0 describing the need to predict failure stress based on the principal stresses and the yield stresses. When any of the local stresses is greater than the specified material ultimate strength; prediction is recommended to be based on the Distortion Energy Theory (DET) or von Mises criteria or on the Maximum Shear Stress Theory (MSST) also known as Tresca yield criterion which states that a part subjected to any combination of loads will fail (by yielding or fracturing whenever the maximum shear stress exceeds a critical value.

Table 7. ANSYS 14.0 predicted failure stresses compared with ultimate stress of material

Properties	NR/UMK/10phr		NR/TSOK/10phr	
	min	Max	Min	Max
x-stress (MPa)	-0.039824	0.066917	-0.003795	0.011386
y-stress (MPa)	0.104955	0.157258	0.7875	0.7875
xy-stress (MPa)	-0.003062	0.002382	-0.07591	0.059041
1 st principal stress (MPa)	0.105019	0.157364	0.7875	0.794038
2 nd principal stress (MPa)	0	0.071242	0	0.010121
3 rd principal stress (MPa)	-0.039888	-0.004432	-0.005612	-0.624E-03
von Mises	0.12965	0.140592	-0.781869	0.791627
Poisson's ratio	0.49		0.47	0.49
Modulus of elasticity			0.02066	
Density				
Shear modulus				
Ultimate strength (MPa)	0.134375		0.7875	

4. CONCLUSIONS

1. The Stress – Strain results of NR/Unmodified kaolin composites are hyperelastic at 2hpr-10phr but NR/TSO modified kaolin composites is more hyperelastic at 10phr.

2. The NR/TSO modified kaolin composite has the Arruda Boyce model fit, the Mooney – Rivlin 9 parameter model fit and Yeoh 3rd order model fit to represent the value of their energy density functions.
3. The NR/Unmodified kaolin composite has its approximate strain energy as 29.12MJ/m³ at 2phr while the NR/TSO kaolin composite has its approximate strain energy as 31.12MJ/m³.
4. von Mises stresses were evaluated to be in the range 0.781869MPa-0.792847MPa.
5. The maximum principal stress is found to be higher than the ultimate tensile strength of 0.7875MPa hence the material is safely specified with load range of von Mises, 0.781869MPa-0.7875MPa.
6. Organomodification of kaolin with tea seed oil (TSO) increases the strength of natural rubber composites.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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