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Numerical and experimental investigation of nanozinc oxide's effect on the mechanical properties of chloroprene and natural rubber (CR/NR) composites

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Nanocomposites, especially natural rubber (NR), have been extensively studied for their unique features and superior performance in tire applications. The present research investigated the impact of zinc oxide nanoparticles (ZnO) on the performance of typical rotary machine seals made of chloroprene rubber / natural rubber (CR/NR) composites. An ordinary standard rubber two-roll mill and hydraulic press were used to prepare high-temperature vulcanized CR/NR samples filled with ZnO nanoparticles. Tensile strength, tear resistance, abrasion resistance, resilience, and hardness were measured to determine the effects of nanoparticles on these physical and mechanical properties. Based on the various hyperelastic modeling schemes, enhancement in multiple characteristics of the control sample, such as overhaul properties, was observed. Furthermore, results show that increasing nanoparticle content in the vulcanisates increased the physicomechanical characteristics, such as hardness, resilience, tensile strength, and elastic Modulus at 200% strain. Moreover, hyperelastic analytical modeling shows that the differences with experimental results are less than 5%.

Keywords: Natural rubber, Chloroprene Rubber, Nanoparticles, Mechanical properties, Hyperelastic models.

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Introduction

Polymers are large molecules composed of repeating subunits called monomers. These monomers are chemically bonded to form a long chain or network structure. Polymers are naturally found in substances like rubber and proteins or chemically synthesized [1]. Rubber is the most popular type of polymer, and it has a wide range of applications across various industries due to its unique properties, such as elasticity, flexibility, High strength and durability, and resistance to wear and tear. Some typical applications of rubber include the automotive, construction, sport, medical industry, consumer goods, etc. [2-4].

Nanocomposite structures refer to materials consisting of two or more components, with at least one part having nanoscale dimensions. These materials combine the unique properties of different features to achieve enhanced functionalities. Fabricating nanocomposite structures involves sol-gel processes, chemical vapor deposition, electrospinning, melt mixing, and in situ synthesis [5]. These techniques allow precise control over the nanoscale additives' size, shape, and distribution within the matrix. Nanocomposite structures have a wide range of applications across industries. They are used in electronics, aerospace, automotive, biomedical engineering, energy storage, and environmental remediation. Examples include high-performance coatings, electronic devices, sensors, biomedical implants, lightweight structural materials, and energy-efficient components. Overall, nanocomposite structures offer the potential to create advanced materials with tailored properties and functionalities, leading to improvements in various technological fields [6].

Conventional nanofillers such as silica, carbon black, and talc are widely used reinforcing agents to enhance the tensile strength and elasticity of the rubber material [7-9]. Metallic nanoparticles such as zinc oxide (ZnO) have attracted broad interest in polymer engineering due to their high stability, good photocatalytic activity, antibacterial activity, and non-toxicity [10,11].

Natural and neoprene rubber should be vulcanized differently; zinc oxide is crucial. Neoprene rubbers are vulcanized with ZnO, whereas natural rubber is vulcanized with ZnO as a vulcanization activator. As a result of ZnO doping, it will be possible to modify the electronic structure of ZnO to tailor its optical, structural, electrical, and magnetic properties. There is an increase in a wide variety of applications due to doping results. These include electronics, spintronics, optoelectronics, photocatalysis, antibacterial treatments, etc. In diverse structures like single crystals, thin films, powders, and nanostructures, ferromagnetic conductivity can be debatable because of its direct band gap energy, luminescence, and high electron mobility [12].

Polychloroprene or neoprene rubber, also called chloroprene rubber, has good physical and mechanical properties resists ozone embrittlement, flexibility and elasticity, and chemical resistance. CR has only a limited range of applications due to its abovementioned properties. Adding fillers can also enhance other properties, such as resistance to physical wear and tear, thermal stability, salinity resistance, and electrical conductivity, enabling CR to be used for various purposes [13].

ASTM International, a recognized global organization, develops and publishes materials, products, systems, and services standards. Many fabrics and products are tested and certified according to ASTM standards. Introducing research papers with ASTM standards can be an effective method of establishing a foundation for the study. Researchers can establish benchmarks, ensure methodological rigor by referencing ASTM standards in the introduction, and compare and validate their results by referencing ASTM standards.

In the vulcanization of neoprene rubber, zinc oxide is used along with magnesium oxide. Two vulcanization routes have been suggested. The first route requires the incorporation of zinc atoms into the crosslink, while the second route leads to ether crosslinks [14].

Due to its nanoparticle size and excellent surface area, nano zinc oxide has been increasingly used to replace conventional zinc oxide in rubber composites in recent years compared to traditional zinc oxide. The multi-atom crosslink precursor is also highly diffused inside diene rubber during compounding and vulcanization processes, allowing it to be in close contact with its atoms.

According to Hiedeman et al. [15], nano zinc oxide produced the same curing characteristics as only a tenth of conventional zinc oxide. Sahoo et al. [16] found that natural and nitrile rubber are more substantial and have a higher crosslink density when nano zinc oxide is used rather than standard zinc oxide. J. Kim et al. [17] found that 1 PHR of nano zinc oxide gives the same cure, mechanical characteristics, and crosslink density as the 5 PHR of traditional ZnO. K. Anand et al. [18] discovered that nano-zinc oxide has a better cure rate index and crosslink density at 0.5 PHR than classical ZnO at 5 PHR, which results in better mechanical properties after aging. Yong Lin et al. [19] investigated the effect of ZnO nanoparticles doped graphene (Nano-ZnO–GE) on NR composites' static and dynamic mechanical properties. It is found that the incorporation of nano-ZnO–GE gives the best cure characteristics of NR compared with the 5 PHR standard compounds of zinc oxide. According to R. A. Nassif et al. (2023), when Nano zinc oxide is added at 2.5%, the highest thermal conductivity (k = 0.677 W/m.°C) and the lowest diffusivity (e = 5.655W/m^2.°C) when compared to other ratios. Adding ZnO to the pure material improves the unsaturated polyester (70%) and nitrile rubber (NR) (30%) composites' thermal stability [20]. Natural waste tire rubber and carbon black were used to make natural-neoprene rubber hybrid composites by P. Kaliyappan et al. [21]. Various percentages of carbon black were used on fabricated composite samples to examine their influences on morphological and mechanical properties.

Several applications were discussed in a review of silicon rubber composites reinforced with carbon nanofillers in 2021 by Kumar et al. [22]. Co-Zn ferrite nanoparticles were used as fillers in silicone rubber composites to enhance magnetization, electric resistivity, and mechanical properties [23]. In their paper, Karthikeyan Suresh et al. (2022) [24] review the effects of nanofillers on chloroprene rubber composite properties and thermal stability. The performance of nanodiamond and nanodiamond/nano-SiO2 hybrid nanoparticles in the tire treads of SBR/BR rubber composites was examined by S. Salkhi et al. (2022) [25]. Xing Xie and Dan Yang (2022) investigated Al_2O_3 nanoparticles' multi-functionalization to enhance the thermal conductivity of epoxy natural rubber composites [26]. Several characterization and analysis studies have been conducted on Ti3C2Tx MXene-Ag/silicon rubber composites [27]. Lastly, Wang et al. [28] conducted a series of non-covalent modified molybdenum disulfide-SiO_2 Nanocomposites (f-MoS_2- SiO_2) fabricated to reinforce hydrogenated nitrile butadiene rubber composites. The effects of nanosheets on mechanical and dielectric properties were studied. Recently, M. Al-Shablle et al. (2022) [29] analyzed the dynamic response of rubber composite nanobeams using two nanoparticles, Al_2O_3 and SiO_2. The experimental and numerical flexural analysis of porous functionally graded polymer beams reinforced by (Al/Al_2O_3) nanoparticles is examined based on various parameters [30]. C. Tan et al. (2023) [31] investigated composites with enhanced electrical and mechanical properties by introducing them into Fluoro Silicone Rubber. Rubber composites are strengthened mechanically by adding different reinforcements. The ultra-small mercaptopropyl doped silica anchored on the Graphene oxide nanosheet has been synthesized to enhance the mechanical properties of nitrile butadiene rubber [32]. According to G. Chen et al. (2023), the design of experiments of Ethylene Propylene Diene Terpolymer (EPDM) was modified by mixing silane with melt and then allowing it to dry out in damp conditions [33]. Xiaoguang Yao et al. [34] studied the cold recycled mixture's mechanical properties and enhancement mechanisms using waterborne epoxy resin/styrene butadiene rubber latex-modified emulsified asphalt.

Moreover, Hassarutai Yangthong et al. (2021) examined the enhancement of cure and mechanical properties of natural rubber vulcanizates by introducing waste wood as filler for rubber materials. 0–3 PHR nano-alumina was incorporated into natural rubber latex foam to investigate the thermal characteristics and kinetics of curing [35]. The influence of Dunlop and air micro bubbling manufacturing methods on nano-Al_2O_3 filled NR latex foam's physical, microstructural, and mechanical properties was investigated using different experimental techniques [36, 37]. In recent decades, nanofillers have been added to enhance chloroprene rubber composites' mechanical properties and thermal stability [38]. Naphon et al. [39] investigated rubber latex's thermal, mechanical, and electrical properties with TiO_2 nanoparticles. Bindu et al. (2013) studied the effect of 5phr conventional ZnO and (0.25, 0.3, 0.4, 0.5, 1,2) phr nano-ZnO on cure characteristics of NR compounds. They found that the compound of 0.5 phr of nano-ZnO is faster in the vulcanization process than that containing 5 phr of conventional ZnO. Also, nano-ZnO with a concentration of 0.5 phr accelerates the vulcanization process and increases the crosslink density [40]. Thomas et al. (2013) studied the effect of conventional ZnO and Nano-ZnO on the mechanical properties of NR. They found that these properties increase by using Nano-ZnO [41]. Consequently, over the past decade, researchers have conducted considerable research on the effects of nanoZnO on rubber composites [42-44]. Subsequently, in rubber composites research, making ZnO nanoparticles dispersed evenly within polymers remains a challenge.

Microparticles of mica waste were produced in the mica mining industry. As per the Dunlop method, natural rubber latex foam composites were characterized by their physicomechanical properties using mica waste loadings ranging from 0 to 10 PHR at 2% intervals. The mechanical properties of Trilene liquid polymers - Ethylene propylene diene monomer (EPDM) containing aramid fibers at five, 10, 15, and 30 PHR in the pulp form were analyzed and carried out [45]. According to Harri Junaedi et al. [46], synthetic hybrid nanocomposites based on short carbon fibers and nanofiller-reinforced polypropylene were studied to see their mechanical and physical properties, compared with mono-filler composites loaded with 15 wt % short carbon fiber, hybrid composites with 15 wt % total filler loading had higher ultimate tensile strength, flexural characteristics, and impact toughness. In Rasana et al.'s study [47], three different nanofillers were evaluated concerning polypropylene composites' microstructure, mechanical properties, thermal properties, and sorption properties. MWCNT and glass fiber composites had tensile strength and a modulus of 79% and 145% higher than neat polypropylene. Based on the literature mentioned above, it was found that characteristics of neoprene composite were not studied before in static and dynamic analysis. This research reports on how varying Nano zinc oxide volume fractions influence the mechanical performance and cure characteristics of CR/NR rubber composites; as a result, these composites could have many associated industrial applications that would benefit from incorporated nanoparticles and improved properties.

I. Experimental work

1.1. Materials

Table 1 summarizes details of the materials used in this study. All materials used in this study were employed in their original state, including various reagents.

1.2. Compound recipes

As shown in Table 2, the matrix of composites used was prepared at different concentrations of Nano zinc oxide [i.e., 0, 0.4, 0.8, 1.2, 1.6, 2, 2.4] PHR.

Table 1.

The materials used in preparing rubber compounds

NO	Material	Properties	Supplier
1	Natural Rubber (NR), (SVR5)		Hoa Thuan CO. Vitnam
2	Neoprene rubber		(GRT) / Vietnam
3	Conventional Zinc oxide	Purity =99 %, size of particle =0.5-1µm, and surface area=3-5m2/gm	ChemTAL SDN-BHD. Malaysia
	Nano ZnO	(size of particle =10-30 nm, surface area=30-60 m2/gm, Assay=99%),	Obtained from the SKYSPRING/ USA.
5	Stearic Acid		Acidchem-International CO. Malaysia
6	Carbon Black	HAF, N660	Iran Carbon CO. Iran
7	Paraffinic Oil		Daura Refinery Iraq
8	CBS		Al-Kiiubar CO. KSA
9	Sulfur		Al-Meshrak CO. Iraq
10	TMQ		Shenyang Sunnyjoint Chemicals CO. China
12	6PPD		Shenyang Sunnyjoint Chemicals CO. China
13	Cyclohexyl-Thio-Phthalimide (CTP-100)		Shenyang Sunnyjoint Chemicals CO. China

1.3. Preparation of Neoprene composites

Various CR/NR composite samples were made through mechanical mixing and hot-pressing. In the beginning, eight samples (S_1- S_8) were prepared according to their constituents, as listed in Table 3. Secondly, using a 20-inch two-roller laboratory mill, the batch for each sample is mixed, and nanoparticles are added. ASTM D-3192 was followed for the melt compounding process.

The next step included using a two-roll mill to add sulfur and MBTS to the compounds for 10 minutes. Two roll-mixing mills were used to prepare the compounds. Their outside diameters were 470 mm, and the speed of the slow roll was 24 rpm.

Finally, the mixture was placed inside a steel mould, and the CR/NR nanocomposite compounds were vulcanized under 15 minutes at 125 °C under 12 MPa using an electrically heated hydraulic press (Moore, England), and the cure times, t90, were determined from the respective cure curves. The same procedure will be followed for each type of the desired test.

The dielectric and mechanical properties of the composites using disc-shaped samples and dumbbell-shaped models with a 25-mm length in a narrow section are also measured. Different properties of vulcanized rubber were calculated, including their tensile strength, elongation, hardness, and Fatigue. All insulation samples were tested under the same conditions based on various parameters. Tests were performed at room temperature and conducted on three models; the results of each test were averaged over three sample preparations.

The Tensometer machine can perform tensile, compression, bending, and other mechanical tests. It has three different load cells (2 KN, 10 KN, and 50 KN) to cover a wide range of measurements. To measure the hardness of rubber according to ASTM D412, the hardness tester ASTM D7121 measures the hardness at 25°C.

Figure 1 depicts the entire experimental procedure used. Vulcanization is essential in rubber composite production to enhance rubber's mechanical properties and improve its performance. Various additives are used in the process that involves heating and pressing rubber. Rubber is strengthened, elastic, chemically, and wear-resistant by vulcanization because cross-links are created between polymer chains. In the current study, the vulcanization processes for test specimens of mechanical properties of neoprene rubber/natural rubber compounds were carried out in the State Company for Rubber and Tires Industries, Iraq, according to ASTM D 3182. The vulcanization process was performed per rheometer test using sheets of approximately 1 mm thickness in a hot press at 150°C. The cured CR/NR composite sheet is trimmed, inspected, and finished per the application's specific requirements. Composite samples are fabricated for achieving hardness, abrasion, resilience, and tensile specimens per ASTM standard, as shown in Figure 2. Table 3 illustrates the Vulcanization technique for preparing NR/CR composite samples.

II. Hyperelastic models

To exploit the simulation of experimental results, the most accurate constitutive models will include compressibility, even though rubbery and elastic materials are incompressible. Finite element codes are used to simulate complex deformations of rubber based on elastic constitutive models. Incompressible material models cause numerical problems that can be avoided through a compressible material model. Compressible materials like rubber are materials that sustain changes in volume under loading. Therefore, these models are better fitting for

Table 2.

The compound recipes of used rubber

Ingredients	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**
NR (SVR5)	50	50	50	50	50	50	50	50
CR (GRT)	50	50	50	50	50	50	50	50
Conventional ZnO	0	0	0	0	0	0	0	5
Nano zinc oxide	0	0.4	0.8	1.2	1.6	2	2.4	0
Pure acid(Stearic)	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0
(TMQ)	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0
(6PPD)	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0
Dry Wax	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0
Carbon black N660	60	60	60	60	60	60	60	60
Paraffinic oil	20	20	20	20	20	20	20	20
MBTS	1	1	1	1	1	1	1	1
Sulfur	3	3	3	3	3	3	3	3
CTP-100	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4

Table 3.

The Vulcanization processes for test specimens

No.	Test-Specimen	Temperature (°C)	Pressure (Mpa)	Time (minutes)
1	Shore Hardness	165	3.2	4.88
2	Tensile Properties and Tear Resistance	145	2.4	45
3	Compression Set	175	2.4	20
4	Abrasion Resistance	178	2.4	20

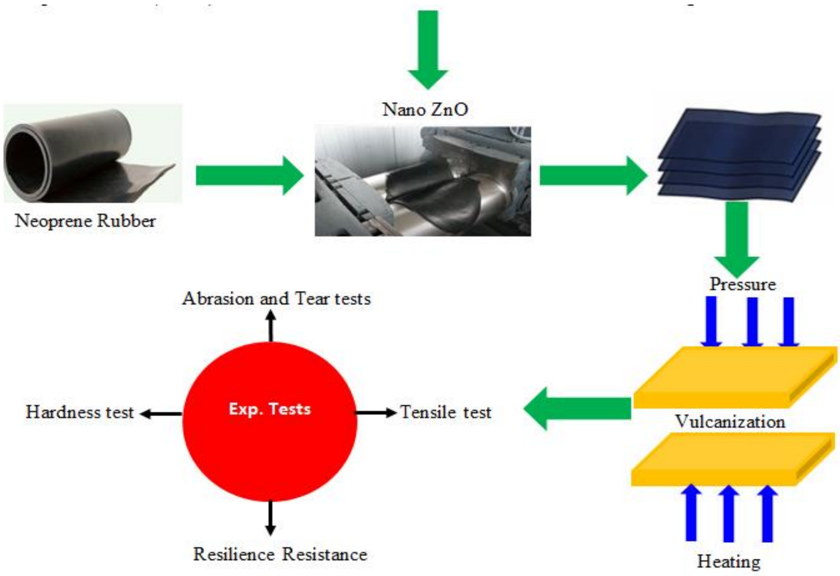

Fig. 1. The preparation process of Neoprene rubber composites and experimental tests.

a b c d

Fig. 2. Samples for tests: a. Tensile test (ASTM D412), b. Tear Test (ASTM 624), c- Hardness and resilience tests (ASTM D7121), d- Abrasion test (ASTM 2228).

researchers, such as rubber, where the results of such modifications [48, 49].

As a sum of terms, Rivlin's general strain-energy function can be expressed for incompressible, isotropic elastic materials.

$$W = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} C_{ij}(I_1-3)^i(I_2-3)^j \quad (1)$$

In the Ogden model, strain energy is expressed as a function of principal stretches φ_1, φ_2, and φ_3. Despite a relatively complex numerical implementation, this model is highly accurate. However, the strain energy function W is:

$$W = \sum_{i=1}^{N}\frac{2\mu_i}{\alpha_i^2}(\varphi_1^{\alpha_i}+\varphi_2^{\alpha_i}+\varphi_3^{\alpha_i}-3) \quad (2)$$

The Arruda-Boyce model, which is written as follows, is another attractive constitutive model:

$$W_{AR} = C_r\sum_{i}^{N} C_i\left(I_1{}^{i}-3^{i}\right) \quad (3)$$

III. Results and Discussion

3.1. Cure Characteristics

The purpose of the rheometer is to determine the strength at which the specimen deforms during vulcanization. Rheometer curves describe changes in strength; hence, composites are evaluated using these curves. As shown in Table 4, conventional and nano zinc oxide incorporated in rubber compound samples are tested for cure characteristics, and values of lower and higher torques are recorded. In terms of maximum torque, the MH-ML exhibits a similar pattern. Furthermore, results indicate that the NR composites' MH, ML, and MH-ML have increased due to the addition of ZnO nanoparticles. The increase in torque values suggests that ENR and filler surfaces interact effectively. One may conclude that the composites' strength comes from the compatibility between ZnO nanoparticles and the NR rubber compounds. The value of the MH-ML can be used to assess the behavior of nanocomposites' crosslink density since it evaluates the dynamic response. The reinforced by ZnO nanoparticles leads to an apparent decrease in scorch, $t_{2,}$ and cure time, t90.

3.2. Material properties

Table 5 summarizes the mechanical testing results of rubber compounds with conventional and nano zinc oxide. From the results presented here, one can conclude that there is an enhancement in most of the mechanical properties with the presence of nanoparticles to a specific limit. Later, those properties will decline.

By boosting the concentration of Nano zinc oxide, which plays a vulcanizing agent role in the vulcanization of chloroprene rubber, the crosslink density of CR/NR composite improves. A higher concentration of Nano zinc oxide improves the mechanical properties by increasing the engagement between the nano zinc oxide duo and the crosslink density. The recorded results indicated that rubber composites are generally vulcanized well using Nano zinc oxide as an activating agent.

Figure 3 illustrates how Nano ZnO affects the tensile strength and elongation of samples of NR rubber composites (S_1 to S_7). As ZnO content in NR composite increases from 0 to 1.2 phr, the material's tensile strength increases from 2.2 to 3.6 (MPa), and its hardness increases from 47 to 58.5. (Shore A). The maximum Tensile strength value is seen in Nano sample S_7 with 7.6 (MPa), while the tensile strength will be minimum at the S_2 sample with zero Nano and conventional ZnO content, and models will show a significant increase again with an increase in Nano ZnO content. This phenomenon can be explained by the fact that the fibers of ZnO Nano are highly resistant to breaking during blending, as it is considered an ideal reinforcement filler. The possible reason for the sharp drop in tensile strength for sample S5 (concentrations of nano zinc oxide 1.6) is that the sample at this Nano ZnO shows low strength, and the internal fiber behaves as a brittle surface.

Using sample S_8 as a reference, it is discovered that when the concentration of Nano-ZnO is between 0 and 0.4 PHR, the tensile strength ranges between 2.2-4.3 Mpa, but it increases to 7.3 Mpa when the concentration of Nano-ZnO = 2 PHR. Nano-zinc oxide samples with 2.4 PHR content have tensile strength equivalent to 7.6 Mpa, similar to rubber composites with 5 PHR conventional zinc oxide.

In nano-zinc oxide at 2.4 PHR, elongation at the break equals 279%, and conventional zinc oxide at 5 phr equals 278%. When the concentration of Nano-zinc oxide is between 0 and 1.6 PHR, the Modulus at 200% varies between (1.7-2.8) Mpa. When the concentration is 2 phr, it increases to 4.8 Mpa. The Modulus at 200% increases to 5.3 Mpa when the concentration of Nano-zinc oxide equals 2.4 phr, whereas the Modulus at 200% is 5.1 Mpa when the activator is the traditional zinc oxide with 5 PHR.

Figure 4 illustrates the hardness and abrasion loss relationship with ZnO nanoparticle content for samples

Table 4.

Rubber compounds cure characteristics of nano (ZnO).

No.	t_{S2} (min.)	t_{90} (min.)	ML (Lb. In)	MH (Lb. In)	MH-ML (Lb. In)	Cure Rate (min.$^{-1}$)
S_1	0.75	1.45	1.28	4.88	3.60	33.333
S_2	0.72	1.40	4.19	6.53	2.34	25
S_3	0.70	1.38	3.79	7.04	3.25	3.030
S_4	0.69	1.36	2.98	7.58	4.6	1.724
S_5	0.67	1.32	3.89	11.73	7.84	1.220
S_6	0.65	1.29	3.88	18.49	14.61	1.064
S_7	0.63	1.26	3.66	19.57	15.91	0.877
S_8	0.55	1.23	3.98	17.26	13.28	0.645

Table 5.

Experimental material characteristics results of NR/CR composites with ZnO nanoparticles

No.	Tensile Strength (Mpa)	Elongation at break (%)	Modulus at 200 % (Mpa)	Hardness (IRHD)	Tear resistance (KN/m)	Abrasion loss (mg/rev.)	Resilience (%)
S_1	2.2	258	1.7	47	14.28	1.6	0.325
S_2	4.3	289	2.9	53	15.3	1.12	1.515
S_3	4.1	287	2.3	55	16.32	1.24	1.952
S_4	3.6	321	2.1	58.5	15.3	0.54	4.203
S_5	3.8	227	2.8	61	18.36	0.7	7.875
S_6	7.3	253	4.8	65	28.56	0.66	35.738
S_7	7.6	279	5.3	66	30.6	0.48	24.853
S_8	7.6	278	5.1	61	25.3	0.33	52.686

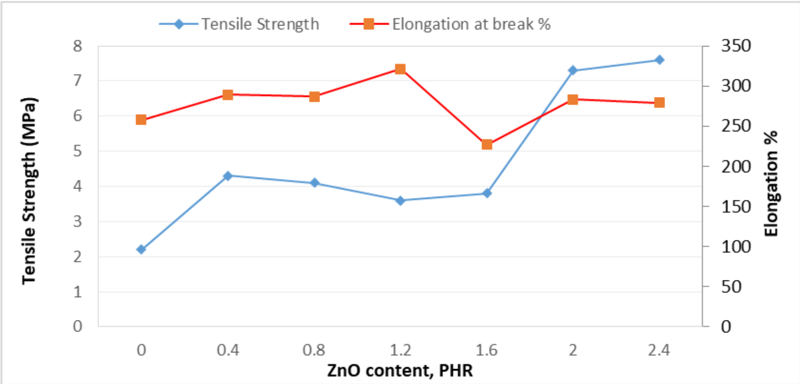

Fig. 3. Effect of Nano ZnO content on CR/NR composites tensile strength and ductility samples.

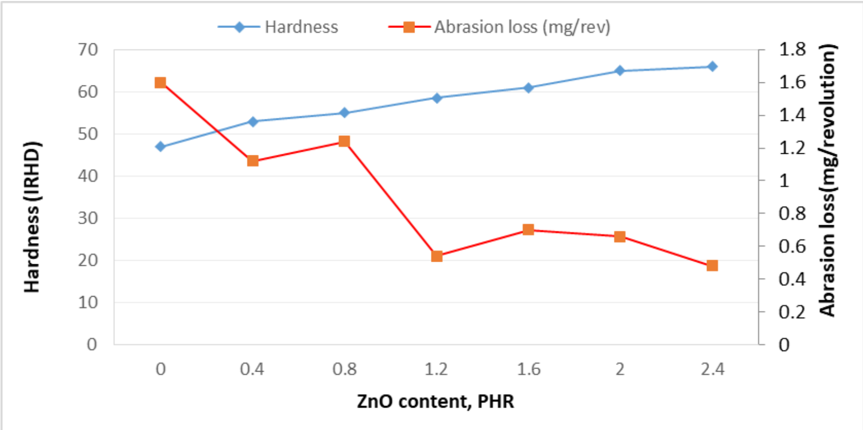

Fig. 4. Effect of Nano ZnO content on CR/NR composite hardness and abrasion loss samples.

S_1 to S_7. This figure shows that an enhancement of those properties was noticed; for example, the hardness increases with increasing Nanoparticles (by changing Nano content from 0 to 2.4, the growth will be 28%). The possible reason is that the reinforcing by Nanoparticles makes the CR composite structure more challenging; hence, the surface resistance to external load increases. The increasing ZnO content from 0 to 1.2 phr in NR composite will decrease the abrasion loss strength from 1.6 to 0.54 (mg/revolution) and hardness from 47 to 58.5 (IRHD). Tear resistance ranges between (14.28-18.36) KN/m when the concentration of Nano zinc oxide is from (0 to 1.6) phr, but it goes up to 28.56 KN/m when the concentration of Nano-ZnO equals 2 phr. It equals 30.6 KN/m at 2.4 phr of Nano-zinc oxide, while the tear resistance equals 25.30 KN/m at 5 phr of conventional zinc oxide. As nano ZnO concentration increases, erosion resistance improves due to the increased property of crosslink density.

Moreover, the best abrasion resistance value equals 0.48 mg/revolution of nano zinc oxide at 2.4 phr and 0.33 mg/revolution of traditional zinc oxide at 5 phr. Due to increased crosslink density, rebound resilience rises as Nano zinc oxide concentration does. When using Nano zinc oxide, the best value for rebound resilience is 35.738%, whereas when using conventional zinc oxide, it is 52.686%.

Based on the above results, one can see that using Nano ZnO instead of classical ZnO decreases the concentration of zinc oxide by 52 %; therefore, using Nano zinc oxide reduces the cost of rubber products, whereas the Nano ZnO and conventional ZnO have similar prices in the international markets. All tested mechanical properties except abrasion loss and rebound resilience improved the hardness by 8.2 %, Modulus at 200 % by 3.92 %, and tear resistance by 20.95 %. These results agree with the studies of Begum [50], Hadi [51], Sahoo [52], and Pornprasit [53].

A comparison and contrast of the present work with prior research illustrating the results of cure mechanical properties using Nano ZnO is presented in Table 6. ZnO is observed to have a better modulus at 200 % by 71.66 % (CR/NR) composites than NR composites, while for elongation at the break, it reduces by 71.89% [16], 29.47 % [51], and 43.14 % [54] in NR composites. In comparison, other research Nano ZnO decreases the tensile strength by 3.94 %, 57.8 %, and 45.825 %. The possible reason for this variation is that the present work uses 2 PHR for CR/NR composites, while Suchismita Sahoo et al. [16] used 3 phr Nano Zno in NR, and F. Hadi and R. Kadhim [51] employed only 2 phr in NR, and finally, S. Q. Mohammed [54] used 2.2 phr of Nano zinc oxide. Furthermore, there are some differences in vulcanization processes for test specimens, reliability of test instruments, and environmental conditions. In this comparison, reinforced rubber proved more resistant to abrasion, wear, and impact than unreinforced rubber. As a result, it exhibits improved strength and durability compared to regular rubber, making it ideal for applications subjected to continuous friction or harsh environmental conditions. Rubber matrix can be reinforced by adding additional reinforcements or reinforcing agents.

Table 6.

Comparison of mechanical properties of the current study relevant to previous studies

Ref.	Hardness (IRHD)	Elong. at break (%)	Modulus at 200 % (Mpa)	Modulus at 300 % (Mpa)	Tensile strength (MPa)
Suchismita Sahoo et al. [16] 3 PHR	-	900 ± 10	1.36 ± 0.03	1.89 ± 0.01	7.6 ± 0.1
F. Hadi, and R. Kadhim [51] 2 PHR	60.333	418	-	10.876	17.303
S. Q. Mohammed [54] 2.2 PHR	-	445	-	9.046	13.475
Present 2 PHR	65	253	4.8	-	7.3

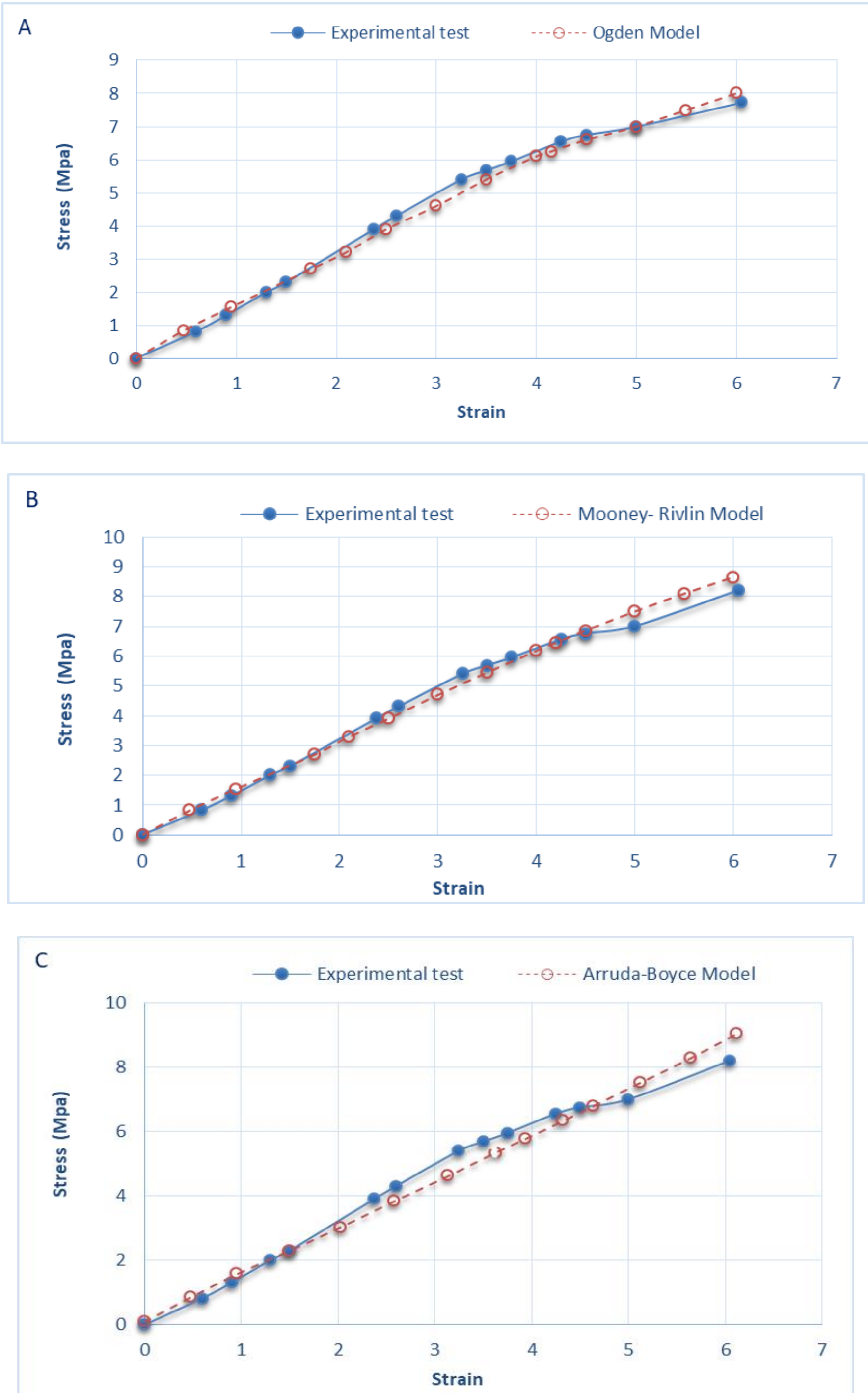

Fig. 5. Stress-Strain curve of 2.4 % ZnO PHR with four hyperelastic models: A) Ogden model, B) Mooney-Rivlin model, C) Arruda-Boyce model.

3.3. Hyperelastic modeling results

Figure 5 illustrates the stress-strain relationship of experimental results with four hyperelastic models (Ogden model, Mooney-Rivlin model, and Arruda-Boyce model) for the sample with 2.4 % ZnO PHR. From this figure, one may conclude that there is a good convergence in results, and the Arruda model represents the best type.

Table 7 further presents coefficient values that apply to a given model. It was done with uniaxial tensile data for sample A8 at 2.4 % Nano reinforcement for predicting mechanical properties. It is found that Ogden's remarkable model can make a 3.5 % fitting error, but the rest of the models predicted parameters with fitting errors of 2.76 %, 25 %, and 28. 5% respectively. This indicates that the Ogden model can represent excellent hyperelastic modeling more than other models.

Table 7.

Parameters of hyperelastic constitutive models for sample S7 (maximum nanoparticles content)

Parameter	Ogden model	Mooney-Rivlin model	Arruda-Boyce model
D	-	-	-
D_1	-	-	-
D_2	-	-	-
$C10$	-	$1.55*10^{-2}$	-
$C01$	-	3.25	-
μ_1	$2.87*10^{-5}$	-	-
α_1	2.99	-	
μ_2	2.46	-	
α_2	-2.71	-	
μ	-	-	$4.45*10^{-2}$
μ_0	-	-	$4.48*10^{-2}$
λ	-	-	2697
Fitting error %	3.5	2.76	28.5

Conclusions

This research examined how ZnO nanoparticles affected the mechanical characteristics of CR/NR rubber composites reinforced with carbon fiber. Regarding the mechanical properties, the results show that ZnO Nanoparticles with 2.4% and zeroes have the same higher tensile strength value as conventional ZnO. Elongation at break (278%) exhibits the same pattern. Because of the use of nanoparticles, the hardness improves by 28.8%. It was also discovered that tear resistance increases with increasing ZnO percentage, with the maximum value being 30.6 KN/m, leading to more significant than the hardness value of zero nanoparticles and 5% conventional ZnO. The abrasion loss value, on the other hand, decreases as the sample's Nano ZnO content increases. The concentration of Nano-zinc oxide increases the hardness. It is equivalent to 61 IRHD at 1.6 phr, comparable to the rubber composite harness at 5 PHR of conventional zinc oxide. It equals 66 IRHD at (2.4) PHR of Nano-ZnO NR and has excellent tensile properties. The filler percolation at 1.2 wt% nanoparticles leads to a marked improvement in the tensile strength to around 9 MPa, while the monotonic response at 3 MPa in the presence of carbon filler percolation could be attributed to carbon filler percolation. The results conclude that rubber can be used in a wide range of industrial applications thanks to vulcanization's improved mechanical and chemical properties.

Three hyperelastic models were used in this study to examine how the Finite Element (FE) simulation of linked materials employs tensile testing. Other models estimate mechanical parameters with high fitting errors, whereas the Ogden model predicts them with approximately 3.5% fitting errors. We have presented the successful fabrication of (CR/NR) Composites using a wide range of experimental tests based on various concentrations of nano ZnO filler. This study also aims to familiarize the user with the recommended procedures in the future and the variables that may be used to influence the outcomes of the designed experiment. Validation tests are strongly advised to gain trust in system design, and precise material property predictions necessitate accurate material properties. Models and detailed material properties for highly extendible materials like rubber composites should be investigated more in future work.

Nomenclature

Symbol	Description
$\mathcal{W}$	Strain energy density
φi (i=1,2,3…)	Stretch ratio
μi	Material constant related to the initial shear Modulus.
αi	Empirically calculated material constants
D, C	Dimensionless material property
N	Order of the polynomial
n	Number of data points
I1, I2,	Principal strain invariants

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Чисельне та експериментальне дослідження впливу нанооксиду цинку на механічні властивості композитів хлоропрену та натурального каучуку (CR/NR)

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Нанокомпозити, особливо природній каучук (NR), ретельно вивчалися на предмет їх унікальних властивостей і прекрасних характеристик у шинах. У цьому дослідженні досліджено вплив наночастинок оксиду цинку (ZnO) на продуктивність типових ротаційних машинних ущільнювачів, виготовлених із композитів хлоропренового каучуку/природнього каучуку (CR/NR). Для приготування високотемпературних вулканізованих зразків CR/NR, наповнених наночастинками ZnO, використовували звичайний стандартний двовалковий млин і гідравлічний прес. Щоб визначити вплив наночастинок на ці фізичні та механічні властивості, вимірювали міцність на розрив, опір розриву, опір стиранню, пружність і твердість. На основі різних схем гіперпружного моделювання спостерігалося покращення багатьох характеристик контрольного зразка, зокрема таких, як властивості відновлення. Крім того, результати показують, що збільшення вмісту наночастинок у вулканізатах підвищило фізико-механічні характеристики, такі як твердість, пружність, міцність на розрив і модуль пружності при деформації на 200%. Гіпереластичне аналітичне моделювання показало, що відмінності від експериментальних результатів становлять менше 5%.

Ключові слова: природній каучук, хлоропреновий каучук, наночастинки, механічні властивості, гіперпружні моделі.