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Mathematical modelling of mechanical properties Polypropylene / Talc composites: Power equation approach

*** Okoye Obuora Anozie, Ntunde Dilibe Ifeanyi**

Department of Mechanical Engineering, Michael Okpara University of Agriculture, Umudike, Abia State, Nigeria

Abstract

The need to comprehend the behavior of engineering materials (Polypropylene/Talc Composites) in order to make detailed selection and use for any kind of product applications necessitated this study. Engineering materials failure can lead to loss of lives, huge loss of capital and wasted effort. In this work, experiments earlier conducted on Polypropylene/Talc composite to determine its mechanical properties (tensile strength, flexural strength and impact strength) were used to mathematically model these mechanical properties of the Polypropylene/Talc composite to produce a *Composite Strength* (in terms of work-done (energy) on the composite and in terms of applied stress on the composite) using the power equation approach. The essence of the model is to produce a linear equation that will inculcate these mechanical properties (tensile strength, flexural strength and impact strength), which are nonlinear, into one mathematical expression with an acceptable R-squared value. Experimental data was modified to have dimensional homogeneity and characterized by multivariate power equations. These mechanical properties were linearized by applying multiple regression analysis to obtain the respective responses of these mechanical properties on the *Composite Strength*. Scatter diagrams were made using Microsoft Excel to affirm the linearized state of the mechanical properties. The mathematical expression presented indicates how each mechanical property of the composite can inhibit or aid the fracture of the sample composite.

Keywords: Power Equation; Tensile Strength; Talc; Polypropylene; Flexural Strength; Nonlinear Model; Microsoft Excel

1. Introduction

Polypropylene (PP) composite is one of the most extensively produced polymers and widely used especially as automotive parts [1]. This is attributed to their high impact strength and toughness when fillers are incorporated.

Polypropylene is isotactic, notch sensitive and brittle under severe conditions of deformation, such as low temperatures or high temperatures. This makes limited its wider range of usage for manufacturing processes. It is a versatile material widely used for automotive components, home appliances, and industrial applications. Polypropylene (PP) filled with particulate fillers is of great interest in both research and industry. It is well known that polypropylene has good processability and accepts different types of natural and synthetic filers. Mica, kaolin, calcium carbonate, and talc are the most often used fillers to reduce both the production costs and to improve the properties of the thermoplastics, such as rigidity, strength, hardness, flexural modulus, dimensional stability, crystallinity, electrical and thermal conductivity. However, fillers have a detrimental effect on other properties such as the impact property and deformability. The filler type, content and size, interfacial adhesion and bond strength between PP matrix and filler and surface characteristics of the composite can greatly influence the filled system.

In a highly filled polymer system, non-uniformity of properties can exist because of poor dispersion of the filler in the matrix. A good interfacial adhesion between matrix and filler may improve the mechanical strength [1-8]. Due to the high transient temperature and in particular, at low stress temperatures, notch toughness of polypropylene is not sufficient and limits its applications. Introduction of fillers or reinforcements into PP often alters the crystalline structure and morphology of PP and consequently results in property changes [5, 9]. Although toughness strength is improved by blending elastomer, this causes a decrease in strength and stiffness [10]. In order to overcome these limitations numerous studies have been performed to improve the toughness, stiffness, and strength balance. Therefore, polypropylene has been modified by different fillers and elastomers to produce ternary composites. The mechanical properties of such ternary composites are determined not only by their composition and the characteristics of the components but also by the phase morphology, and in particular, the relative dispersion of additive components [11].

To meet demanding engineering and structural specifications, PP is rarely used in its original state and is often transformed into composites by the inclusion of fillers or reinforcements.

There are a number of inorganic mineral fillers used with Polypropylene. The most common of these fillers are talc, calcium carbonate and barium sulphate; other mineral fillers used are calcium silicate (wollastonite) and mica (aluminosilicates).

Mineral fillers are generally much less expensive than Polypropylene resin itself. Mineral fillers reduce the costs of the compound formed with Polypropylene and also increase the stiffness. Mineral fillers also provide reinforcement to the polymer matrix as well. Some mineral fillers are surface treated to improve their handling and performance characteristics. Silanes, glycols, and stearates are used commercially to improve dispersion, processing, and also to react with impurities [10].

In this work, the mineral filler used is talc. Hydrated magnesium silicate [$Mg_3Si_4O_{10}(OH)_2$], or better known as talc occurs as the alteration products of magnesium carbonate rock by the natural action of hydrothermal solutions. The purer forms are called steatite talc. The advantages of talc are: Good stiffness, hardness, dimensional stability and reduced creep compared with unmodified PP [12].

Talc can resist temperatures up to 900˚C. It is unaffected by chemicals and will not harm living tissue. Talc can be utilized as a medium filler of average whiteness in thermosetting as well as thermoplastic resins where improvements in electrical insulation, heat, and moisture resistance, chemical inertness and good machinability are needed. Talc has low absorption rate and because of its plate like structure, certain grades can improve flexural properties of mouldings.

In PP, talc gives a good balance of rigidity and impact strength [13]. Advanced milling technology can be used to obtain the finest talc without reducing the reinforcing power of the lamellar structure. Talc filled composites are also easier to colour with reduced pigment require-ment due to its whiteness and low yellow index. Al-though investigations on talc-filled PP have been done since the 1981, there are still many works that involve the characterization of talc filled PP, which are still on-going until today [8].

2. Materials and Methods

2.1 Materials

The grade of Polypropylene used in this work was SEE-TEC Homo polymer PP by LG Chem Korea. This acts as the matrix. The homo polymer PP has a density of 0.90 g/cm3 and a melt flow rate of 14 g/10 minutes (2.16 kg at 230˚C). The nano filler used in this work was Talc (Zeta talc EW 20) manufactured by Eral, Turkey, with particle size of around 2 μm. All the materials were pur-chased from the local chemical market at AjasaOse, Onitsha. The mould release agent used was Petroleum jelly (Vaseline). The characteristic properties of the materials are shown in Table 1.

The nanocomposites were prepared by melting the PP in a mixer and melt compounding it with talc respective-ly at filler loadings of 0%, 5%, 10%, 15%, 20%, 25%, 30% 35% and 40% volume fractions. The tensile samples were cast in an aluminum mould in accordance with ASTM standard D638 for tensile tests, D790 for flexural tests and D256 for impact tests.

Table 1: Characteristic properties of the materials used for the composites

Material	Trade Name	Supplier	Melt Flow Index	Density g/cm3	Melting Temperature ºC	Shape
Polypropylene	SEETEC Homo Polymer	LG Chem Korea	230oC, 2.16 kg/10 min	0.90	170	Pellets
Talc	Zeta talc EW 20	Eral Turkey	-	2.7	-	Powder

2.2 Method of Preparation Manual Mixing and Compounding

The PP was melted from its pelletized form at a temperature exceeding 1800C in a mixing chamber. Measured amounts of Talc were added to the melted PP by volume fractions and stirred continuously for 10 minutes to en-sure a uniform dispersion of the mixture. The com-pounded mixture was cast in an aluminum mould that has been treated with a mould releasing agent and dried. The composite was allowed to cure for 72 hours and was later de-moulded. The composition of composites taken for mechanical tests is shown in Table 2.

2.3 Tensile Testing of the Samples

The tensile experiment was performed on ABBA Universal Testing Machine at a laboratory temperature of 25˚C. The testing machine has rectangular upper and lower grip equipped with centre marking to facilitate the correct positioning of the test specimen when mounted vertically. Tensile testing was performed to determine elastic modulus, ultimate stress, and ultimate strain for all samples. The specimen was prepared and tested in accordance with ASTM D 638.

A minimum of seven samples were tested in each specimen at their various volume fractions. The specimen subjected to tensile test has the dimension 50 × 30 × 20 mm.

Table 2: Combination of composites taken for mechanical tests by volume fractions

Specimen Code	PP %	Talc %
PPT – 0	100	0
PPT – 1	95	5
PPT – 2	90	10
PPT – 3	85	15
PPT – 4	80	20
PPT – 5	75	25
PPT – 6	70	30
PPT – 7	65	35
PPT – 8	60	40

In order to analyze the data, load was converted to stress, σ, from Equation (2.1)

$$\sigma = F/A_0 \qquad (2.1)$$

where F is the force applied as reported from the tensile testing equipment, and A_0 is the original cross sectional area calculated from the average of the sample's neck measurements.

Displacement was converted to millimeters and strain, ε, was calculated using

$$\varepsilon = \Delta l / l_0 \qquad (2.2)$$

where Δl is the change in length of the sample as obtained from the extensometer data, and l_0 is the original extensometer gage length.
The natural strain (or True fracture ductility) is ex-pressed as

$$\varepsilon_n = In^{A_0}/_{A_f} \quad (2.3)$$

where A_0 is the original cross sectional area calculated from the average of the sample's neck measurements and A_f is the Area of the fractured surface.
The Ultimate strength is expressed as

$$\sigma_u = {}^{F_{max}}/_{A_0} \quad (2.4)$$

where F_{max} is the maximum applied force to break the specimen.
Ultimate stress and strain were taken as the maximum values at the sample fracture point, as determined in the data. Results from multiple tests were averaged for each system.

2.4 Flexural Testing of the Samples

Flexural modulus and strength were measured according to ASTM D790 test method with three point bending and was carried out using Instron Universal testing Machine Series XI and support span length was adjusted to 50 mm.
The Flexural Modulus values (E_b) were calculated using the following equation:

$$E_b = {}^{L^3 m}/_{4bd^3} \quad (2.5)$$

where, m is the slope of the tangent to the initial straight line portion of the load-deflection curve.
The Flexural strength (S) in the units of MPa was calculated using the following equation:

$$S = {}^{3PL}/_{2bd^2} \quad (2.6)$$

where P is the applied load at the deflection point, L is the span length, d and b are the thickness and width of the specimen respectively.

3. Methodology

Engineering design variables are often dependent on several independent variables. Often this functional dependence is best characterized by multivariate power equations. A Power Equation model, which is a nonlinear model, is selected to show these obtain a linear relationship. The Power Equation is adopted from [16] as

$$y = \alpha_1 x^{\beta_1} \quad (3.1)$$

Eqn. (3.1) is linearized by taking its base-10 logarithm to become

$$\beta_1 \log x + \log \alpha_1 \quad (3.2)$$

Thus, a plot of *log x* is expected to yield a straight line with a slope of β_1 and intercept of $\log \alpha_1$.
For dimensional homogeneity of three fracture mechanical properties, a basic mathematical theorem was used to transform the yield strength and flexural strength to its energy state or impact strength to its applied stress state. This is achieved by multiplying pressure exerted on the sample composites by the dimensional volume of the sample, to obtain the equivalent work done during both tests (tensile and flexural tests). Likewise, the impact strength is divided by the sample dimensional volume to obtain the equivalent pressure exerted on the test sample. The dimensional volume of the test sample adopted from [6, 15] and used in this evaluation is

$$V = l * b * w \quad (3.3)$$

Where
V = volume of the test sample (rectangular in shape)
l = length of the test sample
b = breadth of the test sample
w = width of the test sample

Now, the power equation to be evaluated is

$$C = A_0 Y^{a_1} F^{a_2} I^{a_3} \quad (3.4)$$

Where
C = Composite Strength
Y = Yield Strength
I = Impact Strength
And a_0, a_1, a_2 and a_3 are coefficients
Taking the logarithm of Eqn. 3.4, the result is

$$\log C = \log A_0 + a_1 \log Y + a_2 \log F + a_3 \log I \quad (3.5)$$

In this form, equation 3.5 is suited for multiple linear regression because ***log C*** is now a linear function of ***log Y, log F*** and ***log I***. Therefore, base-10 logarithm taken of the modified experimental data on Table 3.1 and Table 3.2 and the solutions to Equation 3.5 coefficients are obtained.
The 'best' values of the coefficients are determined by setting the sum of squares of the residuals as

$$S_r = \sum_{i=1}^{n} (C_i - A_0 - a_1 Y_i - a_2 F_i - a_3 I_i)^2 \quad (3.6)$$

Differentiating Equation 3.6 with respect to each of the unknown coefficients

$$\frac{\partial S_r}{\partial a_0} = -2 \sum (C_i - A_0 - a_1 Y_i - a_2 F_i - a_3 I_i) \quad (3.7)$$
$$\frac{\partial S_r}{\partial a_1} = -2 \sum Y_i (C_i - A_0 - a_1 Y_i - a_2 F_i - a_3 I_i) \quad (3.8)$$
$$\frac{\partial S_r}{\partial a_2} = -2 \sum F_i (C_i - A_0 - a_1 Y_i - a_2 F_i - a_3 I_i) \quad (3.9)$$
$$\frac{\partial S_r}{\partial a_3} = -2 \sum I_i (C_i - A_0 - a_1 Y_i - a_2 F_i - a_3 I_i) \quad (3.10)$$

The coefficients yielding the minimum sum of squares of the residuals are obtained by setting the partial derivatives (Eqns. 3.7 – 3.10) equal to zero. This becomes

$$\begin{bmatrix} n & \sum Y_i & \sum F_i & \sum I_i \\ \sum Y_i & \sum Y_i^2 & \sum Y_i F_i & \sum Y_i I_i \\ \sum F_i & \sum Y_i F_i & \sum F_i^2 & \sum F_i I_i \\ \sum I_i & \sum Y_i I_i & \sum F_i I_i & \sum I_i^2 \end{bmatrix} \begin{pmatrix} \log A_0 \\ a_1 \\ a_2 \\ a_2 \end{pmatrix} = \begin{bmatrix} \sum C_i \\ \sum C_i Y_i \\ \sum C_i F_i \\ \sum C_i I_i \end{bmatrix} \quad (3.11)$$

Now, using equation 3.3 and experimental data adopted from [6, 15] to evaluate the yield and flexural strengths of the sample composite in terms of energy absorbed and tabulated in Table 3.1.

Table 3.1: Relating yield, flexural and impact strengths in terms of energy

Composite	Yield Strength, J	Flexural Strength, J	Impact Strength, J
1	876900	1368000	0.13
2	872550	1476750	0.15
3	868200	1585500	0.17
4	834300	1549800	0.195
5	800400	1514100	0.22
6	745950	1449300	0.165
7	691500	1384500	0.11
8	637050	1319700	0.055
9	582600	1254900	0

The solution of equation 3.11 gives the coefficients for a_1, a_2, a_3 and value for $log\ A_0$ as

$$\begin{pmatrix} log\ A_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{bmatrix} 7.843558 \\ -7.97419 \\ 6.494644 \\ 0.325611 \end{bmatrix} \quad (3.12)$$

Since $log\ A_0 = 7.843558$,

then $A_0 = 10^{7.843558} = 6.98 * 10^7$ (3.13)

Substituting coefficients a_1, a_2, a_3 and A_0 into equation 3.4, it becomes

$$C_E = 6.98 * 10^7 * Y^{-7.97} * F^{6.495} * I^{0.33} \quad (3.14)$$

C_E represents the dimensional homogeneity for yield, flexural and impact strengths in terms of work done (energy) on the test sample composite.

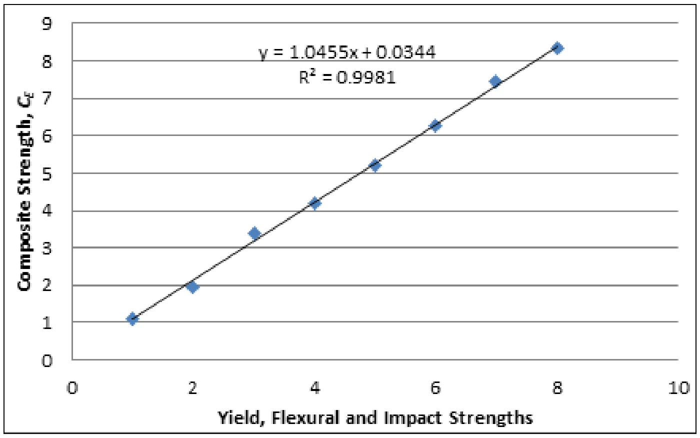

Fig 1: Plot of Composite Strength against Yield, Flexural and Impact Strengths in terms of work done.

Also using equation 3.3 and experimental data adopted from [6, 15] to evaluate the yield and flexural strengths of the sample composite in terms of energy absorbed and tabulated in Table 3.1.

Table 3.2: Relating yield, flexural and impact strengths in terms of applied stress

Composite	Yield Strength, J	Flexural Strength, J	Impact Strength, J
1	29.23	45.60	0.023636
2	29.085	49.225	0.027273
3	28.94	52.85	0.030909
4	27.81	51.66	0.035455
5	26.68	50.47	0.04
6	24.865	48.31	0.03
7	23.05	46.15	0.02
8	21.235	43.99	0.01
9	19..42	41.83	0

Also, the solution of equation 3.11 gives the coefficients for a_1, a_2, a_3 and value for $log\ A_0$ as

$$\begin{pmatrix} log\ A_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{bmatrix} 1.742986 \\ -8.02404 \\ 6.391487 \\ 0.349374 \end{bmatrix} \quad (3.15)$$

Since $log\ A_0 = 1.742986$,

then $A_0 = 10^{1.742986} = 55.33$ (3.16)

Substituting coefficients a_1, a_2, a_3 and A_0 into equation 3.4, it becomes $C_S = 55.33 * Y^{-8.02} * F^{6.39} * I^{0.35}$ (3.17)

C_S represents the dimensional homogeneity for yield, flexural and impact strengths in terms of applied stress on the test sample composite.

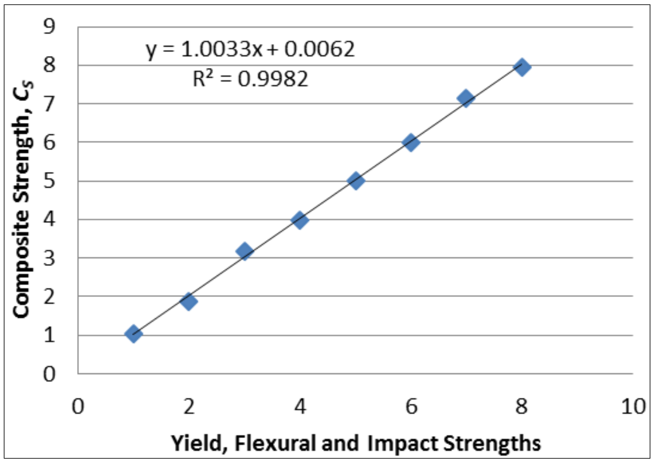

Fig 2: Plot of Composite Strength against Yield, Flexural and Impact Strengths in terms of applied stress

4. Results and Discussion

Fig 1 and 2 provide a linear relationship for yield, flexural and impact strengths in terms of energy and stress applied on the sample composite respectively. The experimental data is used to evaluate the composite strength $\boldsymbol{C_E}$ for both cases. This strength encompasses the yield, flexural and impact strengths. The regression equation of Figures 2 (y=1.0455x+0.0344; R^2 = 0.9981) and Figure 3 (y=1.0033x+0.0062; R^2 = 0.9982) provide a condensed behavior pattern of the nanoparticles in a PP matrix. The R^2 values for C_E and C_S tends towards unity which is very good and this procedure can be accepted for direct product application.

Equations 3.14 & 3.17 are linear relationships developed in order to bring about the linearization of the mechanical properties of a test sample composite which are entirely nonlinear. These linear relationships are termed *OANY* relationships.

5. Conclusions

It has been reported by [6, 15] that the fracture mechanical properties (yield strength, flexural strength and impact strength) and the effect of filler concentration in the PP matrix. Their various properties exhibit different material forms, values and characteristics.

Finally, a mathematical model was developed to relate the yield strength, flexural strengths and impact strengths of a composite material in order to predict the talc filler concentration needed for a particular product application when the minimum fracture mechanical properties for that same particular product application can be estimated. Also, they were tested with other values obtained from similar experiments conducted by different researchers and found to be in good agreement. The *OANY* relationships, $\boldsymbol{C_E = 6.98 * 10^7 * Y^{-7.97} * F^{6.495} * I^{0.33}}$ in terms of work done and $\boldsymbol{C_S = 55.33 * Y^{-8.02} * F^{6.39} * I^{0.35}}$ in terms of applied stress, can be used to evaluate the composite strengths of a Talc/Polypropylene composite for different product applications.

6. References

1. Harikishan M, Sandeep K. Parameter Analysis of Creep models of Polypropylene / Calcium Carbonate Nanocomposites. (Master's thesis, Blekinge Institute of Technology, Karlskrona, Sweden). Retrieved from, 2007 http://essays.se.
2. Manias E. Nanocomposites: Stiffer by Design. Nature material 2007; 6:9-11.
3. Dieter GE. Mechanical Metallurgy 1, metric edition. Boston, M.A: McGraw Hill, 1988.
4. Karger-Kocsis J. Microstructural aspects of fracture in polypropylene and in its filled chopped fibre and fibre material reinforced composites. In Polypropylene. Structure, Blends and Composites; Karger-Kocsis, J., Ed.; Chapman and Hall: London, UK 1995; 3:142-201.
5. Mgbemena CO. Evaluation of the Mechanical properties of Polypropylene/Calcium Carbonate nanocomposites at various creep conditions. (Masters' thesis, Nnamdi Azikiwe University, Awka, Nigeria), 2010.
6. Okoye OA. Fracture Mechanical Behavior of Polypropylene/Talc Composites. (Master's thesis, Nnamdi Azikiwe University, Awka, Nigeria), 2011.
7. Pukánszky B. Particulate filled polypropylene: Structure and properties. In Polypropylene, Structure, Blends and Composites; Karger-Kocsis, J., Ed.; Chapman and Hall: London, UK. 1995; 3:1-70.
8. Pukánszky B. Fillers for polypropylene. In Polypropylene. An A-Z reference; Karger-Kocsis, J., Ed. Kluwer Academic: Dordrecht, The Netherlands, 1999, pp. 240-246.
9. Ferrigno TH. Principles of filler selection and use. In Handbook of Fillers and Reinforcements for Plastics; Katz, H.S., Milewski, J.V., Eds.; Van Nostrand Reinhold: New York, NY, USA, 1987, pp. 8-62.
10. Weidenfeller B, Höfer M, Schillling F. Cooling Behaviour of Particle Filled Polypropylene during injection moulding process. Composites: Part A 2005; 36:345-351.
11. Friedrich K, Karsch UA. Failure processes in particulate filled polypropylene. J. Mater. Sci. 1981; 16:2167-2175.
12. Qiu Y, Lin Z, Mai K. Fracture of Mg(OH)2/Polypropylene composites modified by functionalized polypropylene. J. Appl. Polym. Sci. 2002; 88:2148-2159.
13. Nielsen LE, Landel RF. Particle-filled polymers. In Mechanical Properties of Polymers and Compo-sites; Marcel Dekker: New York, NY, USA, 1993, pp. 377-450.
14. Móczó J, Pukánszky B. Polymer micro and nanocomposites: Structure, interactions, properties. J. In-dust. Engin. Chem. 2008; 14:535-563.
15. Mgbemena CO, Okoye OA. Computational Approach to Modelling Fracture Behaviour of Polypropylene/Talc Composites. Journal of Materials and Materials Characterisation and Engineering. 2012.
16. Chapra SC, Canale RP. Numerical Methods for Engineers, Sixth Edition, McGraw Hill Education (Asia) Inc. Singapore, 2010, pp. 467-468.
17. Kissel WJ, Han JH, Meyer JA. Polypropy-lene: Structure, properties, manufacturing and applications. In Handbook of Polypropylene; Karian, H., Ed.; Marcel Dekker AG: Basel, Switzerland, 2003, pp. 10-27.
18. Zhuk AV, Knunyants NN, Oshmyan VG, Topolka-raev VA, Berlin AA. Debonding Microprocesses and Interfacial strength in particle-filled polymer materials. J. Mater. Sci. 1993; 28:4995-5606.
19. Theocaris PS, Demakos CB. Crack propagation modes in particulates: A study approaching reality. J. Compos. Mater. 1988; 22:154-176.
20. Guth EJ. Theory of Filler Reinforcement. Journal of Applied Physics. 1945; 16:20-25.