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Prediction of the Elastic Properties of Ultra High Molecular-Weight Polyethylene Particle-Reinforced Polypropylene Composite Materials through Homogenization

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Abstract: In this study, to improve the mechanical properties of polypropylene (PP) with the objective of developing a composite with ultra-high-molecular-weight polyethylene (UHMWPE) as a reinforcement, the mechanical properties of the composite material were investigated via numerical analysis and finite element analysis (FEA). Based on a mathematical approach, the modulus of elasticity, shear modulus, and Poisson's ratio were calculated using a numerical model, and, through FEA with application of the homogenization method, the elastic properties were predicted, and the results were comparatively analyzed. In the future, it will be necessary to compare experimental and numerical analysis results to verify the findings of this study.

Keywords: UHMWWPE; polypropylene; finite element analysis; composites; polymer

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1. Introduction

With the ongoing advancement of industrial society, the demand for high-rise, long-span, and large building structures is increasing, leading to increases in the performance, strength, and functionality of such structures. In accordance with this trend, high-quality, new composite materials and applications of cutting-edge structural engineering technology are being actively developed. In addition, recent research on the development of composite materials has focused on achieving multifunctionality and reducing the weight of such materials, and numerous studies have been conducted to improve the mechanical properties of the existing polymer materials. Basically, the reinforcement mechanisms of polymer composite materials can be classified into two types. The first method is particle reinforcement using powder. In this approach, by using graphene oxide [1–4] and specially prepared coating powder [5–8], the isotropic properties of the existing polymers can be improved. The second technique is fiber reinforcement, in which carbon nanotubes [9–12], carbon fibers [13–16], or various other materials are added to synthesize anisotropic composite materials. These materials have drawbacks in terms of difficulties in prediction and analysis based on classical theories due to the complex interplay among the bending-tensile, tensile-shear, and bending-torsion effects. Challenges informing the use of these materials have also been reported. To address these limitations, more in-depth research on isotropic composite materials is required. In the context of the research objectives for isotropic composite materials described above, ultra-high-molecular-weight polyethylene (UHMWPE) has emerged as an attractive option. This material has been one of the most relevant for total hip and knee replacements over the last 50 years [17] and has emerged as the material of choice for fabricating bearing components in various arthroplasties, such as acetabular cups, tibial inserts, and glenoid sections [18,19]. Furthermore, due to the high tensile

strength, wear resistance, and strength-to-weight ratios of UHMWPE fibers, UHMWPE is considered an excellent reinforcement material [20–22]. However, in general, UHMWPE is a fiber-type reinforcement. The fiber-reinforcing material may be classified as an anisotropic material, and, since the injection moldability is low, a disadvantage of processing occurs. To apply it to various industries, development of an isotropic UHMWPE-PP material suitable for injection molding is required. In this study, a composite material obtained by mixing UHMWPE and PP in powder form was proposed. Accordingly, the change in elastic properties according to the addition of UHMWPE was theoretically estimated. To develop isotropic composite materials by using UHMWPE with excellent properties in powder form and mixing the powder with the existing polymer material, polypropylene (PP), the elastic properties can be predicted through finite element analysis (FEA). Therefore, in this study, to predict the elastic properties of UHMWPE-particle-reinforced PP composite materials, FEA was performed with different volume fractions (2, 4, 6, 8, 10, and 15 VF%) of UHMWPE with a size of 10 μm. The FEA results were compared to those of the conventional model for numerical analysis.

2. Numerical Analysis Model

The rule of mixture (ROM) is a well-established analytical method for evaluating the elastic properties of materials. The following equation is utilized to evaluate elastic properties using the ROM [23,24]. There are two methods of determining the mechanical properties of composite materials: using the weight fraction (W%) or volume fraction (VF%) of the reinforcement and the matrix for the composite material. The ROM calculation is performed based on the volume fraction of the components of the composite. In practical applications at industrial sites, the weight fraction method is easier because most manufacturing equipment for composite materials employs a gravimetric system for material supply. However, to perform numerical analysis for the elastic properties of the reinforcement and matrix, the volume fraction is used for calculation. The equations for calculation of the elastic properties are as follows:

$$E_c = E_R \times V_R + E_M \times V_M \tag{1}$$

$$V_R + V_M = 1 \tag{2}$$

E_C : prediction modulus of elasticity of composite material;
E_R : modulus of elasticity of reinforcement material;
V_R : volume fraction of the reinforcement;
E_M : modulus of elasticity of matrix material;
V_M : volume fraction of the matrix.

In addition, numerous effective medium approximations have been developed to predict the effective elastic moduli of two-component composite materials consisting of particles embedded in a matrix [25]. Hobbs used the volume fraction of reinforcement and developed an effective medium approximation for the predicted modulus of elasticity (Ec) of a two-component mixed composite material based on the moduli of elasticity of the reinforcement and matrix.

$$E_c = E_M \left[1 + \frac{2V_R(E_R - E_M)}{(E_R + E_M) - V_R(E_R - E_M)} \right] \tag{3}$$

In this study, the results of the two numerical analysis methods described above were compared with the FEA results.

3. Homogenization Method

Homogenization techniques have received increasing attention for predicting the mechanical properties of composite materials over the past decades [26–28], because homogenization techniques can efficiently quantify the interplay between microscopic and

macroscopic properties [29–31]. In this study, to predict the effective values of the elastic properties of composite materials, representative volume elements (RVE) were composed according to the UHMWPE volume fraction using specialized software (Ansys Material Designer), and the changes in the effective elastic properties of the material according to the UHMWPE volume fraction were comparatively analyzed using a numerical approach.

To develop a numerical model required for the homogenization method, UHMWPE was applied as the particle-reinforced material, and a spherical shape with a diameter of 10 μm was used for modeling. The material for the matrix was PP, considering the size of the particle-reinforced material. As shown in Figure 1, the matrix was modeled as a cube with dimensions of 40 μm × 40 μm × 40 μm. In addition, to reflect the fact that UHMWPE was present as particles inside the cube-shaped matrix, an RVE model with an irregular arrangement of the particles was developed. The use of homogenized material data significantly lowers the computational cost of composite simulations, as the structure only needs to be simulated on a macroscopic scale.

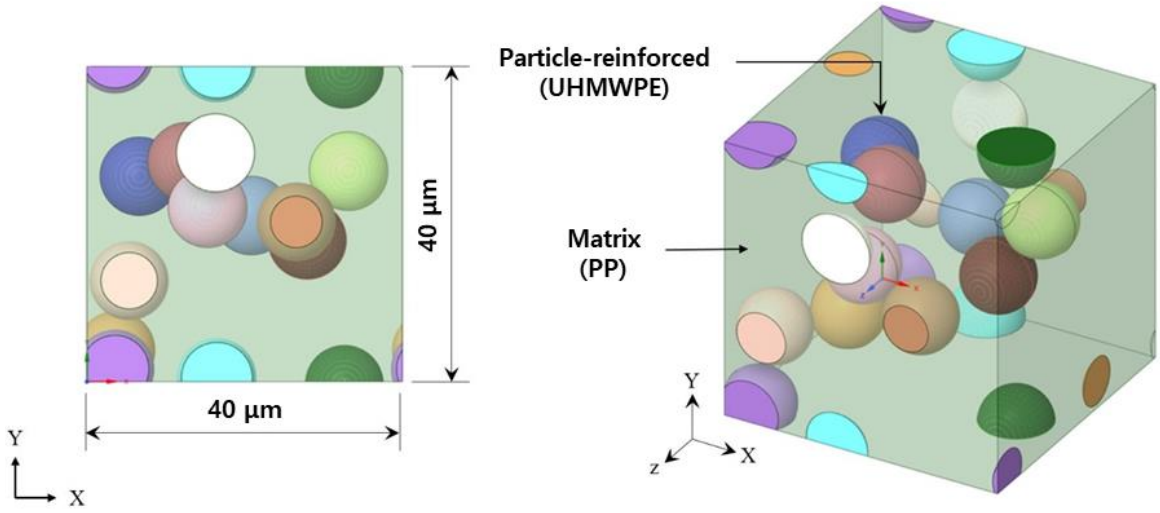


Figure 1. UHMWPE-particle-reinforced PP composite employed for RVE modeling.

The mesh size of the RVE model with an increased volume of UHMWPE-particle-reinforced material was increased to 2 μm, and the numerical models with different volume fractions are presented in Figure 2. The models consisted of the arrangement of randomly formed UHMWPE according to the volume fraction. The modeling algorithm of the random deployment of UHMWPE was as follows. To minimize variability in physical properties in composites due to excessive random arrangement, it was set that the powder of UHMWPE was added based on the existing 2% (VF). Therefore, although the random arrangement of UHMWPE was constructed, it was expected that interpretation with a certain tendency would be performed. The node and element information are summarized in Table 1.

Table 1. Number of elements in finite element analysis.

	Unit	2%	4%	6%	8%	10%	15%
Node	Ea	113,767	113,211	118,315	119,491	121,788	127,324
Element	Ea	79,752	79,468	82,908	83,584	85,213	88,649

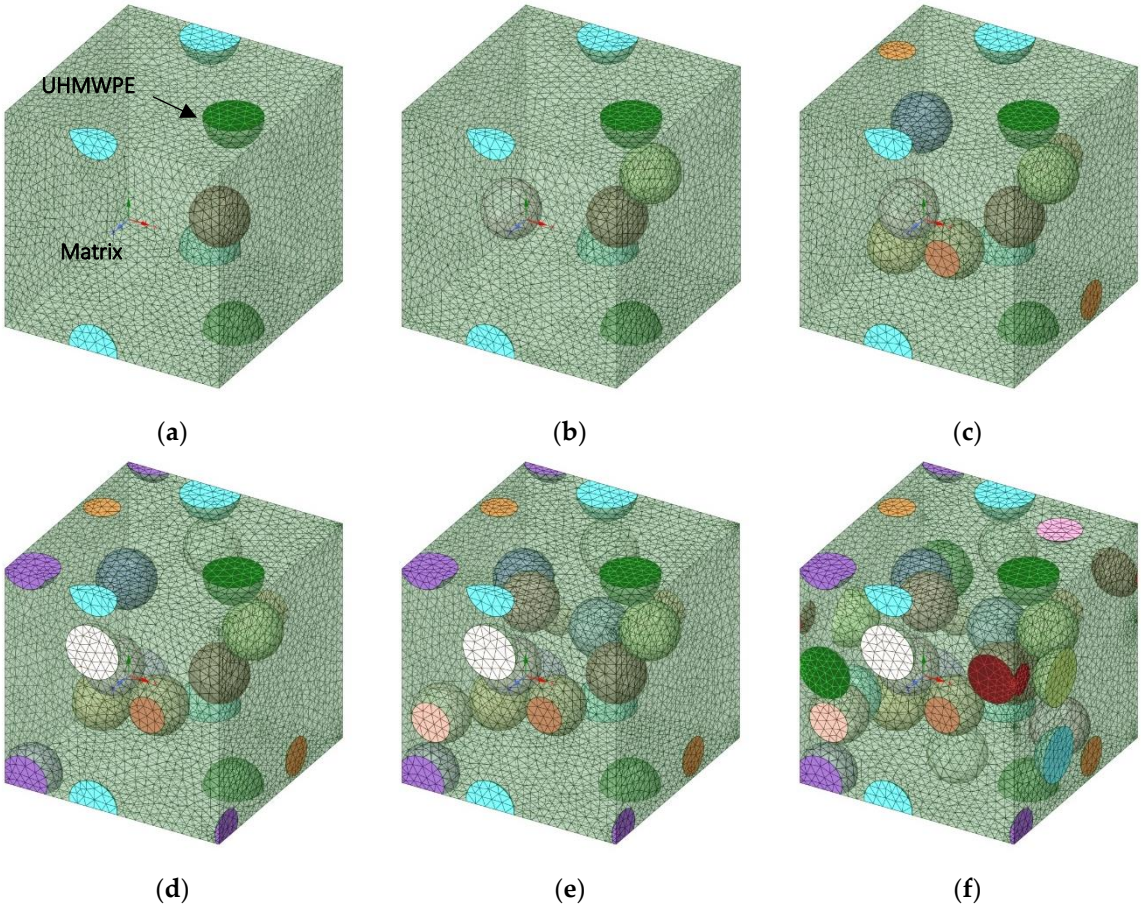


Figure 2. Mesh modeling with UHMWPE volume fraction. (**a**) 2%. (**b**) 4%. (**c**) 6%. (**d**) 8%. (**e**) 10%. (**f**) 15%.

In addition, the mechanical properties of the PP and UHMWPE used for this analysis are summarized in Table 2. The numerical approach and FEA method enabled prediction of the elastic properties of the mixture according to the volume fraction based on the basic properties of PP and UHMWPE presented below.

Table 2. Properties of PP and UHMWPE.

	PP	UHMWPE
Modulus of elasticity (MPa)	1325	25,000
Shear modulus (MPa)	432.29	10,417
Poisson's ratio	0.43	0.20
Bulk modulus of elasticity (MPa)	3154.8	13,889.0
Density (kg/m^3)	904	950

Because the difference between the moduli of elasticity of the PP and UHMWPE used in this study was large, it can be judged that the higher the volume fraction of UHMWPE, the higher the modulus of elasticity of the mixture. In addition, considering that the Poisson's ratio of UHMWPE was 0.2 and that of PP was 0.43, it was expected that the Poisson's ratio of the mixture would be lower than 0.43.

4. Results

The numerical analysis results and the finite element analysis results are shown in Tables 3 and 4. In the numerical approach employed in this study using the ROM method,

the predicted modulus of elasticity of the composite material with a UHMWPE volume fraction of 2% was 1789.6 MPa. With increasing volume fraction, the predicted modulus of elasticity also increased, and, at a volume fraction of 15%, the modulus of elasticity was 4876.3 MPa, corresponding to an increase of 270%. The shear modulus was also shown to increase up to 1930.0 MPa as the volume fraction of UHMWPE increased. The reason for the increase was determined to be as follows. With the modulus of elasticity of UHMWPE being 25,000 MPa and that of PP being 1325 MPa, the difference between the moduli of elasticity of these materials was considerable; however, the calculation was performed by simply considering the changes in the volume fraction. On the other hand, by predicting the elastic properties using the Hobbs equation, as shown in Equation (3), an increase in the modulus of elasticity from 126% to 1738.2 MPa was obtained at a 15% volume fraction of UHMWPE. The shear modulus was increased by 126%. We now present a comparison of the elastic properties between the results predicted using a numerical analysis model and those obtained by FEA.

Table 3. Numerical analysis result.

Model	Contents	Unit	2%	4%	6%	8%	10%	15%
ROM model	E11	MPa	1798.5	2272.0	2745.5	3219.0	3692.5	4876.3
	G11	MPa	632.0	831.7	1031.4	1231.1	1430.8	1930.0
	nu12	-	0.43	0.42	0.42	0.41	0.41	0.40
Hobbs equation	E11	MPa	1373.5	1423.9	1476.2	1530.4	1586.9	1738.2
	G11	MPa	448.5	465.3	482.8	501.0	519.9	570.8
	nu12	-	0.42	0.42	0.41	0.41	0.40	0.39

Table 4. Finite element analysis results.

Model	Contents	Unit	2%	4%	6%	8%	10%	15%
FEM	E11	MPa	1392.80	1439.30	1519.50	1572.80	1661.90	1851.70
	E22	MPa	1396.60	1458.20	1538.10	1600.30	1685.70	1882.60
	E33	MPa	1392.80	1439.30	1515.60	1570.10	1670.80	1865.40
	G12	MPa	487.06	506.20	532.20	550.73	582.11	644.55
	G23	MPa	487.24	504.67	528.38	547.80	577.89	648.52
	G31	MPa	488.16	505.43	535.16	554.68	587.48	657.72
	nu12		0.43	0.42	0.42	0.41	0.42	0.41
	nu13		0.43	0.43	0.43	0.43	0.42	0.42
	nu23		0.43	0.43	0.42	0.42	0.42	0.41

Table 4 presents the predicted values of the elastic properties calculated using FEA. By performing FEA, the modulus of elasticity, shear modulus, and Poisson's ratio were calculated for the direction of each RVE axis. It was judged that these values were within the error range. Because the UHMWPE powder used as reinforcement was assumed to have a spherical shape, according to the characteristics of the particle-reinforced isotropic composite materials, the material was considered as an isotropic composite material. For comparison of the mechanical properties predicted using FEA with those obtained from the numerical analysis, the average values of the elastic properties calculated according to the direction of each axis were compared with the numerical analysis results. The predicted modulus of elasticity of the isotropic composite material with 2% UHMWPE calculated through FEA was 1394.1 MPa, which was similar to the numerical calculation result using the Hobbs equation rather than that obtained by using the ROM. The same trend was

observed as the volume fraction of UHMWPE increased. To determine this trend clearly, a comparative analysis was conducted using the graphs shown in Figure 3.

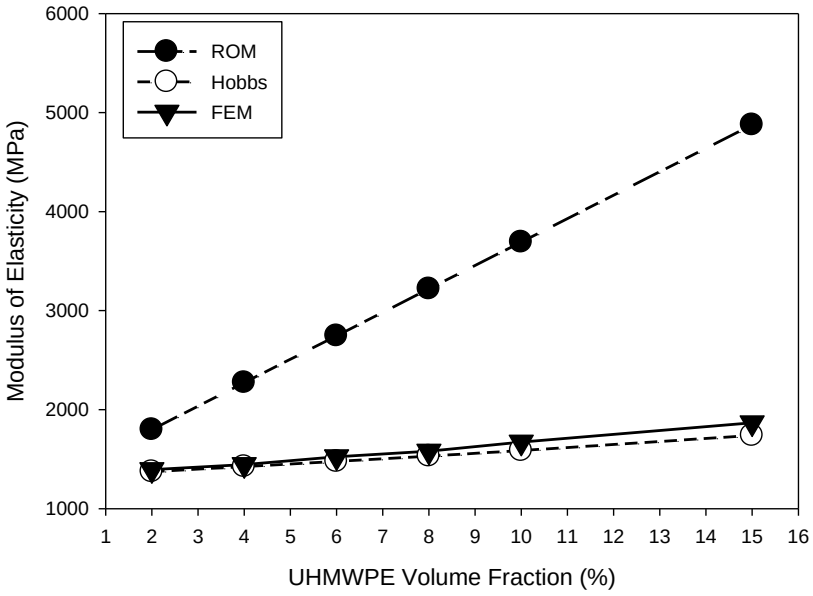


Figure 3. Comparison of modulus of elasticity.

The predicted modulus of elasticity of the PP-UHMWPE mixture is shown in Figure 3. Basically, because the modulus of elasticity of UHMWPE was approximately 19 times higher than that of PP, it can be considered that the higher the volume fraction of UHMWPE, the higher the modulus of elasticity of the mixture. For quantitative comparison of the difference between the predicted moduli of elasticity, the elastic index (EI) was calculated. The EI of the modulus of elasticity predicted using the ROM method was 236.8 MPa/vf%, that obtained using the Hobbs equation was 28.1 MPa/vf%, and that calculated by the finite element method (FEM) was 36.3 MPa/vf%. The shear modulus in Figure 4 is also expressed in terms of the shear index (SI) for quantitative comparison of the results. The SI of the shear modulus predicted using the ROM method was 99.8 MPa/vf%, that obtained from the Hobbs equation was 9.4 MPa/vf%, and that calculated by the FEM was 12.5 MPa/vf%. From these results, it can be judged that, in the prediction of the modulus of elasticity and shear modulus using the ROM model, the difference between the results obtained by FEM and the ROM model continued to increase with increasing volume fraction because the EI and SI were large. In general, the ROM model is linearly calculated according to the volume fraction of the reinforcing agent of the composite material, as shown in Equation (1); thus, as the volume fraction increased, the excellent physical properties of UHMWPE were linearly reflected, and the elastic properties increased. Additionally, since the elastic modulus of UHMWPE was 25,000 MPa, which is higher than the 1325 MPa of PP, the composite material was more elastic depending on the volume fraction. On the other hand, in the Hobbs equation, the physical properties are determined according to the volume fraction of the reinforcing agent, and the elastic modulus of the base material and the reinforcing agent is calculated by combining them. According to these estimation methods, there was a difference compared to the ROM model. As shown in Figure 5, because the Poisson's ratio of UHMWPE was smaller than that of PP, the Poisson's ratio decreased with the increasing volume fraction of UHMWPE.

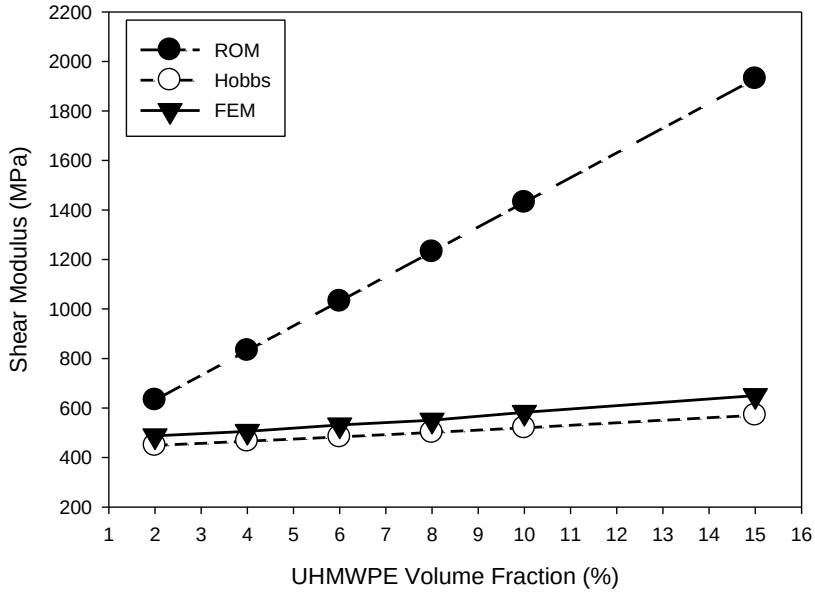


Figure 4. Comparison of shear modulus.

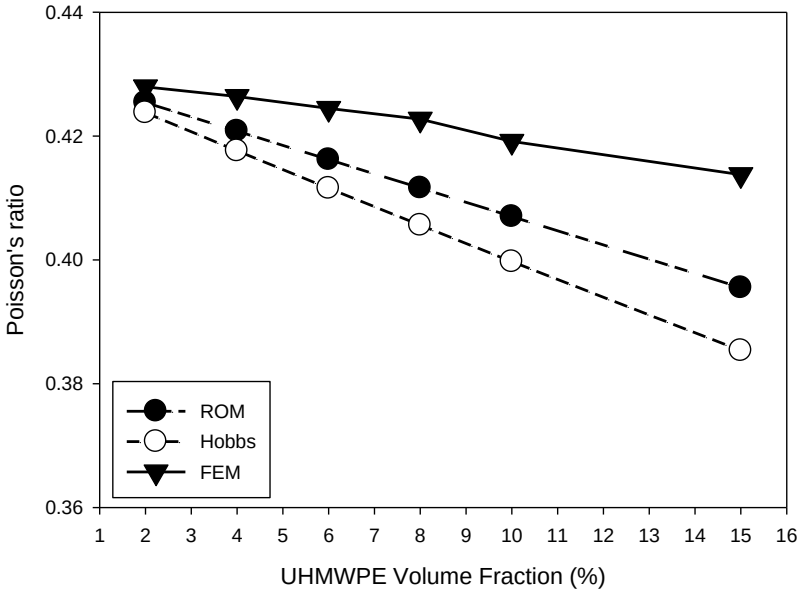


Figure 5. Comparison of Poisson's ratio.

In this study, a composite reinforcing existing PP using UHMWPE particles was developed, and a numerical approach was employed to predict the elastic properties of the composite. Numerical calculations were performed using the ROM model and Hobbs equation, and the results of comparative analysis using FEA confirmed that the error was large in the case of the ROM model. Further, a trend in the values of the elastic properties similar to that of the FEM values was obtained using the Hobbs equation.

5. Conclusions

In this study, we predicted the elastic properties of a composite material using UHMWPE powder as reinforcement and PP as a matrix, using numerical analysis and the FEM to investigate the mechanical properties of the composite. As a result of applying UHMWPE powder for reinforcement, the PP-UHMWPE powder composite was modeled as an isotropic material, and the values of the elastic properties were comparatively analyzed according to the volume fraction of UHMWPE. The numerical analysis was

performed using the ROM model and Hobbs equation, and the FEM results were employed for comparison based on the homogenization method using RVEs. The key findings of this study can be summarized as follows:

(1) The elastic properties predicted using the ROM model according to the volume fraction of each material showed large errors;
(2) The elastic properties predicted based on the Hobbs equation were similar to those obtained using the FEM, and the change trends of the elastic properties according to the volume fraction were also similar between the two sets of results;
(3) In the prediction of the elastic properties with an isotropic composite prepared using reinforcement material with a spherical shape or in the form of a fine powder, the Hobbs equation produced results with a more similar trend to the FEA results than the ROM model did, and the former method is more appropriate for applications involving isotropic composite materials.

In the future, it will be necessary to conduct further research on the prediction of the elastic properties of isotropic composites with high volume fractions of UHMWPE, and additional investigation is required for optimization of the volume fraction. In addition, finite element analysis and numerical analysis should be quantitatively compared and analyzed based on the experiment.

Further, experimental studies involving the preparation of real-world PP-UHMWPE composites are required, as well as research on the factors that could be adjusted to minimize the errors among the real-world experimental results, numerical analysis results, and FEA results.

Author Contributions: Conceptualization, J.-H.Y.; Writing—original draft, Y.-J.J.; Writing—review & editing, writing—original draft preparation, supervision, M.-S.K. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

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