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Optimization of Graphene Oxide's Characteristics with TOPSIS Using an Automated Decision-Making Process

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Abstract. The present study focuses on a new application of TOPSIS to predict and optimize graphene oxide's characteristics. Although this carbon-based material has been investigated previously, its optimization with this method using an automated decision-making process has not been performed yet. The major problem in the design and analysis of this nanomaterial is the lack of information on comparing its characteristics, which has led to the use of diverse methods that have not been appropriately compared. Moreover, their advantages and inconveniences could be investigated better once this investigation provides information on optimizing its candidates. In the current research work, a novel automated decision-making process was used with the TOPSIS algorithm using the Łukasiewicz disjunction, which helped detect the confusion of properties and determine its impact on the rank of candidates. Several characteristics of graphene oxide, such as its antibiofilm activity, hemocompatibility, activity with ferrous ions in hydrogen peroxide, rheological properties, and the cost of its preparation, have been considered in its analysis with TOPSIS. The results of this study revealed that the consideration of the criteria of this nanomaterial as profit or cost criteria would impact the distances of candidates from the alternatives. Moreover, the ranks of the candidates changed when the rheological properties were considered differently in the data analysis. This investigation can help improve the use of this nanomaterial in academic and industrial investigations.

Keywords: process innovation, energy optimization, prediction, TOPSIS, algorithm.

1 Introduction

Graphene oxide (GO) is a substantial two-dimensional nanomaterial that was prepared using the oxidation of graphene after the discovery of this nanomaterial by Novoselov et al. in 2004 [1]. It is among the carbon-based materials with various applications in science and engineering [2].

The physical properties of GO are comparable with those of graphene by removing the functional groups from its surface. The presence of the functional groups makes GO hydrophilic and dispersable in water, whereas graphene has hydrophobic properties [2].

Different GO sizes from nm to mm can be obtained using different sonication periods [3]. The optimization of the characteristics of GO is an important procedure required for the improvement of its design and manufacture.

2 Literature Review

The physicochemical, mechanical, and biological characteristics of GO, such as its activity with ferrous ions in hydrogen peroxide [4], rheological properties [5], antibiofilm activity [6], hemocompatibility [7, 8], and the cost of its preparation [9] with or without polymers have been carried out, previously. These properties of GO were chosen in this investigation for their optimization with the Technique for Order of Preference by Similarity to the Ideal Solution (TOPSIS). As indicated in the mentioned studies, the GO production with the less defective reduced product was performed in hydrogen peroxide [4], and the indicated properties significantly impacted the quality of GO [5]. Moreover, the practical value of GO was revealed in killing bacteria related to its surface physical properties [6]. It has been revealed that the interactions between the hematological entities, such as blood cells, and GO would influence the efficacy of its biomedical applications [7].

It is worth noting that the production of GO using less costly procedures for energy storage and conversion applications would be required [8]. The consideration of these properties of GO can lead to the energy optimization of its design and preparation.

The thickness of a single-layer GO flake measured with atomic force microscopy typically ranges between 1.0 nm and 1.4 nm [10, 11], which is above the thickness value measured for graphene (0.7 nm [12]). The thickness of GO can change according to its preparation procedure. No detailed investigation on the impact of the thickness of GO on its correlative characteristics has been done yet. Therefore, its thickness has not been considered for optimization in the current study.

TOPSIS is a method that considers the profit and cost criteria and optimizes the candidates. This has been done by considering their distances from the alternatives for comparative analysis using different methods [13], decision-making processes [14], and financial performance evaluation [15]. All these analysis procedures have included the advantages of TOPSIS. Universality is an advantage of this method [16]. The simplicity of computation and presentation is its other advantage [17].

The selection of the best process for removing color with the use of adsorbent materials [18], the improvement of the GO dispersion properties [19], the selection of graphene oxide nanocomposites [20], the optimization of the mixture proportions of graphene oxide [21] and the evaluation of the performance on reduced graphene oxide synthesized [22] have been performed with the TOPSIS method. However, no study has been done on the optimization of the physicochemical, mechanical, and biological characteristics of GO previously. For the first time, the optimization of this nanomaterial based on these characteristics is investigated in the current paper.

The objectives of this study have been to determine the results of the optimization of the characteristics of GO. For this, the unmodified and modified TOPSIS methods have been used.

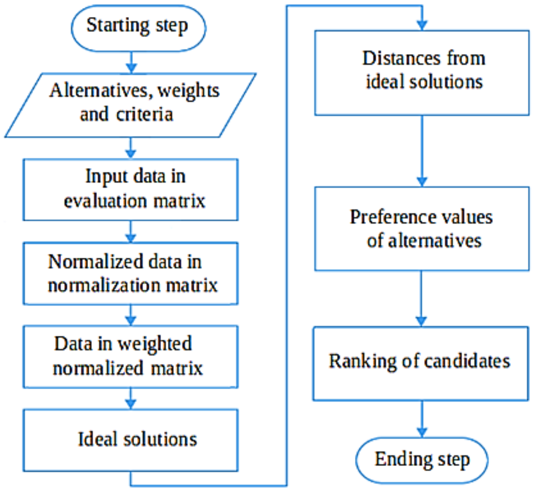
The results of this study reveal the impact of the criteria of this nanomaterial as profit or cost criteria on the distances of each candidate from the alternatives. The ranking of the candidates can be affected by different considerations of its characteristics in several analyses. This investigation can help improve the use of this nanomaterial for further applications in science and engineering.

3 Research Methodology

3.1 TOPSIS method

The following TOPSIS algorithm in Python was used for the optimization of GO: https://github.com/Glitchfix/TOPSIS-Python/blob/master/topsis.py.

Figure 1 presents the flowchart of the steps of the unmodified and modified TOPSIS methods. The modification step in the evaluation matrix, including the Łukasiewicz disjunction, does not exist in the unmodified TOPSIS algorithm but is used in its modified version.



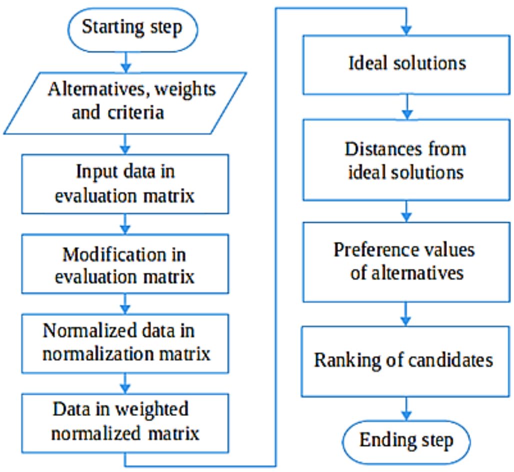


Figure 1 – The flowchart of the research steps with unmodified (a) and modified (b) TOPSIS

The other steps are in common in the two procedures. The Łukasiewicz disjunction in the modified TOPSIS method enables the algorithm to perform automated decision-making to distinguish the categories of graphene-based materials.

The activity of GO with ferrous ions in hydrogen peroxide [4], its rheological properties [5], antibiofilm activity [6], hemocompatibility [7, 8], and the cost of its preparation [9] have been optimized with TOPSIS in the current study.

The results with TOPSIS were obtained as described previously for data pre-processing [23] and ranking similarity [24].

3.2 Modified TOPSIS

The modified TOPSIS using the Łukasiewicz disjunction optimized the GO candidates with a novel automated decision-making process. This method sets the maximum value acceptable in the TOPSIS algorithm to 1.0. Therefore, this procedure detected and analyzed the confusion in considering the GO properties. The modified TOPSIS algorithm was required to determine how the rank of the GO samples would change when the individual confused their properties with those of the other graphene-based samples, such as the reduced GO.

4 Results

Table 1, in three parts, shows the terms, their corresponding values of fuzzy membership degrees for the properties of GO samples, and their average values.

Table 1 – Terms, their related membership degrees of the characteristics of GO samples, and average values

Candidates/ criteria	Antibiofilm activity	Hemo compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	low	medium	medium	low	low
C_2	medium	medium	medium	medium	medium
C_3	medium	low	high	medium	high
Values of the characteristics					
Candidates/ criteria	Antibiofilm activity	Hemo-compati-bility	activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.2, 0.3, 0.4	0.4, 0.5, 0.6	0.4, 0.5, 0.6	0.2, 0.3, 0.4	0.2, 0.3, 0.4
C_2	0.4, 0.5, 0.6	0.4, 0.5, 0.6	0.4, 0.5, 0.6	0.4, 0.5, 0.6	0.4, 0.5, 0.6
C_3	0.4, 0.5, 0.6	0.2, 0.3, 0.4	0.7, 0.8, 0.9	0.4, 0.5, 0.6	0.7, 0.8, 0.9
Average values					
Candidates/ criteria	Antibiofilm activity	Hemo compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.3	0.5	0.5	0.3	0.3
C_2	0.5	0.5	0.5	0.5	0.5
C_3	0.5	0.3	0.8	0.5	0.8

The weight value of 0.5 is chosen for the criteria. In the next step, the criteria matrix of GO samples is determined. In the criteria matrix, all the characteristics of GO, apart from its cost, are considered as profit criteria. This last one is considered as a cost criterion. Therefore, the terms "true" and "false" are indicated in this matrix for the first and last criteria, respectively.

In the next step, the vector normalization of data for the GO samples is performed.

Tables 2, 3 show the results of the normalization procedure and the multiplication of weights with the normalized data, respectively.

The determination of the alternatives is performed in the next step. Table 4 shows the values of the alternatives for GO samples.

Table 2 – Data in normalized decision matrix

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.3906	0.6509	0.4683	0.3906	0.3030
C_2	0.6509	0.6509	0.4683	0.6509	0.5051
C_3	0.6509	0.3906	0.7493	0.6509	0.8081

Table 3 – Data in weighted normalized decision matrix

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.0781	0.1302	0.0937	0.0781	0.0606
C_2	0.1302	0.1302	0.0937	0.1302	0.1010
C_3	0.1302	0.0781	0.1499	0.1302	0.1616

Table 4 – The alternatives for GO samples

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
A^+	0.1302	0.1302	0.1499	0.1302	0.0606
A^-	0.0781	0.0781	0.0937	0.0781	0.1616

The distances from the alternatives for the GO samples are obtained in the next step.

Table 5 shows the values of distances from the alternatives for GO samples.

Then, we performed the analysis of the similarity coefficients of the GO samples.

Table 6 shows the similarity coefficient (CC_i) values and the ranking of the GO samples according to their worst similarity.

Table 5 – The distances from the alternatives for GO samples

Candidates	d_i^*	d_i^-
C_1	0.0926	0.1136
C_2	0.0692	0.1087
C_3	0.1136	0.0926

Table 6 – CC_i and the ranking of GO samples

Candidates	CC_i^*	Ranking
C_1	0.5509	2
C_2	0.6109	1
C_3	0.4491	3

Figure 2 shows the results of Table 6. The values of the distances from the best and worst alternatives and similarity coefficients (CC_i) of the GO samples are presented in black, red, and green, respectively.

Considering that the rheological properties of GO samples could be their cost criteria, the term "false" was chosen for these properties instead of the term "true" in the criteria matrix of the GO samples. Tables 7 to 11 show the results obtained with the TOPSIS method after this modification.

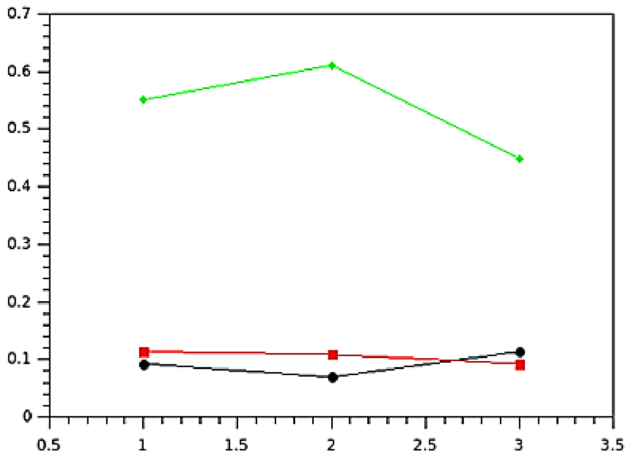


Figure 2 – The values of the distances from the alternatives and similarity coefficients (CC_i) of GO samples

Table 7 presents the data of the normalized decision matrix for the GO samples. Table 8 presents the data of the weighted normalized decision matrix for the GO samples.

Table 9 presents the alternatives for the GO samples. Table 10 shows the distances from the alternatives for the GO samples. Table 11 shows the similarity coefficient values and the ranking of the GO samples.

Figure 3 shows the results of Table 11.

Table 7 – Data in the normalized decision matrix

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.3906	0.6509	0.4683	0.3906	0.3030
C_2	0.6509	0.6509	0.4683	0.6509	0.5051
C_3	0.6509	0.3906	0.7493	0.6509	0.8081

Table 8 – Data in the weighted normalized decision matrix

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.0781	0.1302	0.0937	0.0781	0.0606
C_2	0.1302	0.1302	0.0937	0.1302	0.1010
C_3	0.1302	0.0781	0.1499	0.1302	0.1616

Table 9 – The alternatives for GO samples

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
A^+	0.1302	0.1302	0.1499	0.0781	0.0606
A^-	0.0781	0.0781	0.0937	0.1302	0.1616

Table 10 – The distances from the alternatives for GO samples

Candidates	d_i^*	d_i^-
C_1	0.0766	0.1250
C_2	0.0866	0.0954
C_3	0.1250	0.0766

Table 11 – CC_i and the ranking of GO samples

Candidates	CC_i^*	Ranking
C_1	0.6200	1
C_2	0.5241	2
C_3	0.3800	3

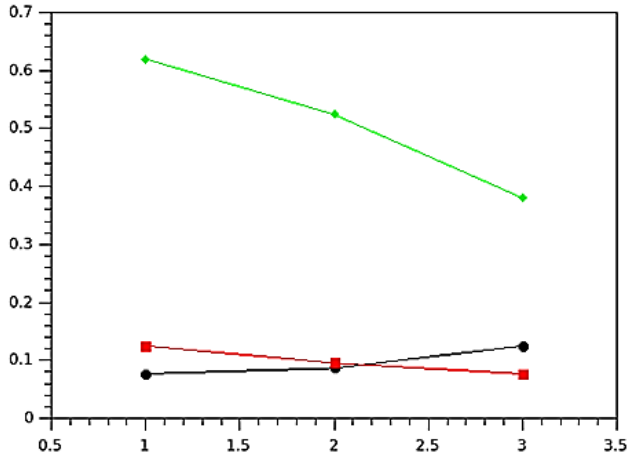


Figure 3 – The values of the distances from the alternatives and similarity coefficients (CC_i) of GO samples

The values of the distances from the best and worst alternatives and similarity coefficients (CC_i) of the GO samples are presented in black, red, and green, respectively.

As revealed by the obtained results in this paper, the ranking of the GO samples is influenced by modifying the consideration of their characteristics as profit or cost criteria. In the first ranking, the ranks 2, 1, and 3 were obtained for the first, second, and third candidates. In the second series of analysis, when these nanomaterial's rheological properties were considered cost criteria, the ranks 1, 2, and 3 were obtained for the first, second, and third candidates, respectively. Moreover, the values of distances from the alternatives and those of their similarity coefficients that determined their ranks also changed following this modification.

In another series of analyses, the modified TOPSIS algorithm with the Łukasiewicz disjunction was used to optimize the GO candidates with an automated decision-making process. In the analysis with the modified TOPSIS, the maximum value of the cost of GO in the evaluation matrix obtained in the algorithm's output for candidates 1 and 3 was 1.0. No other change was performed in the optimization. The data in the criteria matrix were like the ones used in the previous analysis.

Table 12 shows the results of the normalized decision matrix for the GO samples. Table 13 shows the results of the weighted normalized decision matrix for the GO samples.

Table 14 shows the values of the alternatives for the GO samples. Table 15 shows the values of distances from the alternatives for the GO samples. Table 16 shows the GO samples' similarity coefficients (CC_i) and ranking.

Table 12 – Results of the normalized decision matrix

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.3906	0.6509	0.4683	0.3906	0.6667
C_2	0.6509	0.6509	0.4683	0.6509	0.3333
C_3	0.6509	0.3906	0.7493	0.6509	0.6667

Table 13 – Results of the weighted normalized decision matrix

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
C_1	0.0781	0.1302	0.0937	0.0781	0.1333
C_2	0.1302	0.1302	0.0937	0.1302	0.0667
C_3	0.1302	0.0781	0.1499	0.1302	0.1333

Table 14 – The alternatives for GO samples

Candi-dates/ criteria	Antibiofilm activity	Hemo-compati-bility	Activity in hydrogen peroxide	Rheological properties	Cost
A^+	0.1302	0.1302	0.1499	0.0781	0.0667
A^-	0.0781	0.0781	0.09365858	0.1302	0.1333

Table 15 – The distances from the alternatives

Candidates	d_i^*	d_i^-
C_1	0.1016	0.0736
C_2	0.0766	0.0993
C_3	0.0993	0.0766

Table 16 – CC_i and the ranking of GO samples

Candidates	CC_i^*	Ranking
C_1	0.4203	2
C_2	0.5646	3
C_3	0.4354	1

Figure 4 shows the results of Table 16. The values of the distances from the best and worst alternatives and similarity coefficients (CC_i) of the GO samples are presented in black, red, and green, respectively.

The obtained results in the last series of analyses showed that the ranks of the GO samples depended on the values of their properties in the evaluation matrix.

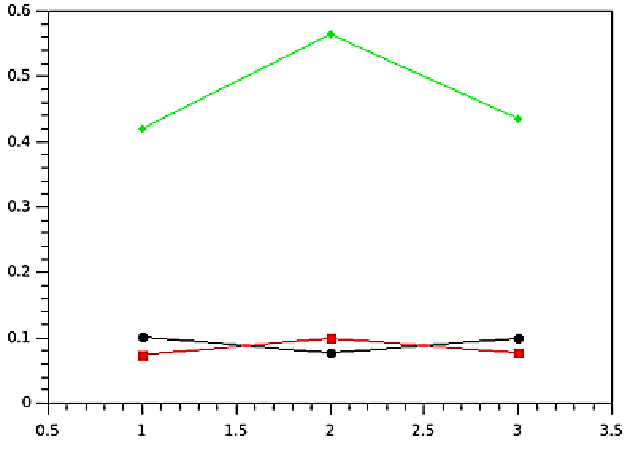


Figure 4 – The values of the distances from the alternatives and similarity coefficients (CC_i) of GO samples

Figure 5 shows the values of the distances from the alternatives and similarity coefficients (CC_i) of the first-ranked GO samples of the three series of analyses. The results for the first, second, and third analyses are represented in the left, middle, and right, respectively.

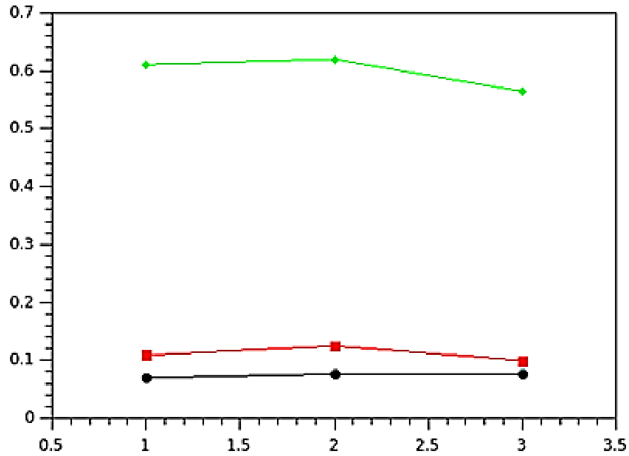


Figure 5 – The values of the distances from the alternatives and similarity coefficients (CC_i) of the first-ranked GO samples of the three series of analyses

As shown in Figure 5, the lowest value of d_i^* and the highest value of d_i^- were observed for the first-ranked candidates of the first and second series of analyses, respectively. Moreover, the highest value of CC_i was observed for the first-ranked sample of the second analysis.

Further comparison of the obtained results showed that the distances of the GO samples from their ideal solutions and their ranks depended on the use of modified and unmodified TOPSIS algorithms. In the first series of analyses using the unmodified TOPSIS method, the second, first, and third samples had the first, second, and third ranks, respectively. In the second analysis series, when GO's rheological properties were considered cost criteria, the first, second, and third samples had the first, second, and third ranks, respectively. However, in the third series of analyses using the modified TOPSIS method, the second, third, and first samples had the first, second, and third ranks, respectively. These results showed the effect of the Łukasiewicz disjunction in the change of the ranking of candidates.

5 Discussion

The comparison of rankings obtained with the unmodified and modified TOPSIS methods revealed that the rank of the GO samples could change with the automated decision-making process using modified TOPSIS due to the confusion of the categories of samples by the individual. This showed that when the individual confused the properties of the GO samples with those of other graphene-based samples, this could change the ranks. Moreover, the results of ranking the GO samples obtained with the modified TOPSIS algorithm differed from both results obtained in the first and second series of analyses with unmodified TOPSIS.

The physical [25, 26], chemical [27, 28], and biological properties [29, 30] of different nanomaterials have been investigated in recent years. Further investigations are required for the optimization of the properties of these materials with TOPSIS.

The thickness of GO can have impact on the efficiency of certain devices such as solar cells [31]. Recently, the effects of the thickness of GO on some of its properties such as its friction [32] and hydrogen production [33] have been reported. However, these properties have not been correlated, yet. More investigations are required to optimize the correlated characteristics of this nanomaterial.

The current study, as the first optimization of the characteristics of GO using unmodified TOPSIS and an automated decision-making process with the modified algorithm, can help a better understanding of the characteristics of this nanomaterial for its further design and applications.

6 Conclusions

This paper presented for the first time the optimization of the chemical, rheological and biological characteristics and the cost of GO using the TOPSIS method. Two algorithms, umodified and modified, were used in several series of analyses.

The impact of the characteristics such as the antibiofilm activity, hemocompatibility, activity with hydrogen peroxide, rheological properties, and the preparation cost of this nanomaterial on the candidates' ranking was investigated.

In the first series of analysis with unmodified TOPSIS, the vaues of the similarity coefficient of the first, second and third GO samples were 0.61, 0.55, and 0.45, respectively. These values in the second series of analysis with unmodified TOPSIS were 0.62, 0.52, and 0.38, respectively. In the third series of analysis with modified TOPSIS, the values were 0.44, 0.42, and 0.56, respectively.

The ranks of candidates were done according to these values, which helped optimize the samples considering their characteristics. The results obtained in this paper showed that the modification in the type of criteria would modify the ranks related to the changes in the values of the candidates' distances from the alternatives and those of their similarity coefficients. These results can be used for the comparative optimization of nanomaterials with applications in science and engineering.

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