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Analysis of Nanoparticles Characteristics with TOPSIS for Their Manufacture Optimization

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Abstract. The present study focuses on the comparative analysis of superparamagnetic iron oxide nanoparticles (SPIONs) characteristics with the TOPSIS method. The prediction of the characteristics of SPIONs is required for better manufacturing of these nanoparticles. Although the characteristics of these nanoparticles have been investigated, no research has been done on their comparison in order to determine which one of their surface functionalities would be more appropriate for their diverse applications. The objective of this study was to analyze the characteristics of SPIONs without or with surface charge with a prediction model and TOPSIS in order to determine the best nanoparticles. Moreover, the effect of inappropriate consideration of their cost criterion on their ranks was explored with the modified TOPSIS. This analysis showed that the characteristics of SPIONs such as antibiofilm activity, hemocompatibility, activity with hydrogen peroxide, rheological properties, and the labour of their chemical synthesis could affect their ranking. Neutral SPIONs, negatively charged SPIONs, and positively charged SPIONs were ranked as the first, second, and third candidates, respectively. However, the improvement of the activity of positively charged SPIONs with hydrogen peroxide showed an increase to 0.3 instead of 0.2, which resulted in a better rank of these nanoparticles in comparison with that of the same nanoparticles in the first analysis series. One of the advantages of this study was to determine the impact of the characteristics of SPIONs on their ranking for their manufacturing. The other advantage was getting the information for further comparative study of these nanoparticles with the others. The results of this work can be used in manufacturing engineering and materials science.

Keywords: SPIONs, chemical activity, biological properties, rheological properties, TOPSIS, industrial growth, manufacturing engineering.

1 Introduction

Superparamagnetic iron oxide nanoparticles (SPIONs) have diverse applications such as magnetic drug targeting, magnetic hyperthermia, photocatalytic applications, etc. For most materials science and engineering applications, these nanoparticles are suspended in water [1–3]. The characteristics of SPIONs that were first studied in recent investigations have been as follows: antibiofilm activity, hemocompatibility, activity with hydrogen peroxide, rheological properties, and labour for their chemical synthesis in the lab [4–8].

The antibiofilm activity and hemocompatibility studies of SPIONs require the assessment of these nanoparticles with biological materials, which are bacterial biofilms and blood cells (ex.: red blood cells and platelets), respectively [4, 5, 9–14]. These analyses of SPIONs have allowed the development of their applications in materials science and biomedical engineering [15–20].

The Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) is a decision-making method that allows optimizing and ranking candidates. This method has been widely used to analyze candidates, such as electronic devices, cognitive entities, etc. Hwang and Yoon developed TOPSIS in 1981 to determine solutions from a finite set of alternatives [21, 22]. TOPSIS ranks candidates according to their distances from their ideal solutions with the consideration of their profit and cost criteria [21–26].

This paper considers these characteristics of SPIONs: antibiofilm activity, hemocompatibility, activity with hydrogen peroxide, rheological properties, and labour for their chemical synthesis. The first four properties of these nanoparticles are positive because their increase is beneficial for their biomedical and engineering applications, whereas the last one is negative because less labour would be more appropriate in order to spend less time and energy on the chemical synthesis of these nanoparticles. Therefore, in this study, the first four indicated properties were considered as profit criteria and the last one as cost criterion.

TOPSIS has been used to analyze the properties of some materials and those of human beings according to their traits [27–32]. It has also been used to rank manufactured devices and instruments [33–38].

The analysis of the characteristics of SPIONs for optimizing their manufacture with TOPSIS has not been reported yet. This paper's results can be used to improve the applications of these nanoparticles in materials science and biomedical engineering.

2 Research Methodology

2.1 Preparation of SPIONs

The neutral, positively charged, and negatively charged SPIONs studied in this work were the nanoparticles prepared according to the protocols described in previous studies [4, 5, 6, 7, 39].

2.2 TOPSIS method

The TOPSIS code that Chakravorty developed in 2016 (https://github.com/Glitchfix/TOPSIS-Python/blob/master/topsis.py) was used for this analysis.

The numerical analysis with TOPSIS was carried out on two groups of characteristics of SPIONs; positive and negative characteristics were considered profit and cost, respectively.

The steps of the TOPSIS method were as below [40–46] :

Step 1: Creation of a normalized decision matrix

The normalized R decision matrix was created in step 1 according to the formula below:

$$r_{ij} = \frac{X_{ij}}{\sqrt{\sum_i^m = 1^{x_{ij}^2}}}$$

Step 2: Creation of a weighted normalized decision matrix V

This matrix was created using the formula below:

$$v_{ij} = w_j . r_{ij}$$

Step 3: Determination of the positive ideal solution (A^+) and the negative ideal solution (A^-)

The positive ideal solution (A^+) and negative ideal solution (A^-) were calculated with the TOPSIS method as described previously [40, 41, 42].

Step 4: Calculation of the separation distance from the positive ideal solution S^+ and the other distance from the negative ideal solution S^- for each candidate

These distances were calculated using the formulas below:

$$D_j^* = \sqrt{\sum_{i=1}^{n} (v_{ij} - v_i^*)^2}, \ j = 1,\ldots,J.$$

$$D_j^- = \sqrt{\sum_{i=1}^{n} (v_{ij} - v_i^-)^2}, \ j = 1,\ldots,J.$$

Step 5: Calculation of the similarity coefficients using the proximity relative to the ideal solution

The candidates' similarity coefficients were calculated with the formula below:

$$C_j^* = \frac{D_j^-}{D_j^* + D_j^-}, \ j = 1,\ldots,J.$$

The ranking according to the value of closeness coefficient (C_j^*) was described previously [47–54].

2.3 Modification of TOPSIS

The TOPSIS code was modified with the formulas below according to the Lukasiewicz's type disjunction:

```
self.evaluation_matrix[self.row_size-2][self.column_size-1]=self.evaluation_matrix[self.row_size-2][self.column_size-1] + 0.6

self.evaluation_matrix[self.row_size-3][self.column_size-1]=self.evaluation_matrix[self.row_size-3][self.column_size-1] + 0.6

if self.evaluation_matrix[self.row_size-2][self.column_size-1]>1:

self.evaluation_matrix[self.row_size-2][self.column_size-1]=1
if self.evaluation_matrix[self.row_size-3][self.column_size-1]>1:

self.evaluation_matrix[self.row_size-3][self.column_size-1]=1
```

These lines added to the first step in the TOPSIS code will add the value of 0.6 to the mean values of the membership degrees of the properties of neutral and positively charged SPIONs in the last column (labour of chemical synthesis), the first and second rows of Table 1. As the previous values of these membership degrees were 0.4, their summation with 0.6 will give 1.0, and the maximal value according to Lukasiewicz's type disjunction is 1.0. Therefore, these modifications in the TOPSIS code will make the values of 1.0 for these membership degrees in Table 1.

3 Results and Discussion

The results obtained in this study are included in the steps below:

1. Determine the mean values of triangular fuzzy membership degrees of candidates' characteristics.

The terms and corresponding triangular fuzzy values of the membership degrees of the characteristics of SPIONs and their mean values are shown in Table 1. The information about SPIONs as three candidates, C-1, C-2, and C-3, with their different characteristics, is presented in the table. Antibiofilm activity, hemocompatibility, activity with hydrogen peroxide, and rheological properties, which positively affect the candidates' properties as they reveal the efficiency of their activity, are profit criteria. The last one, the labour of their chemical synthesis, has a negative effect on this output as less labor for their manufacture is desired. So, this characteristic is considered a cost criterion. The mean values of fuzzy membership degrees of the candidates' characteristics according to the chosen terms (low, medium, or high) are indicated in the table.

Table 1 – Terms and their corresponding triangular fuzzy values of membership degrees of characteristics of SPIONs and their mean values

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
C-1	medium	medium	low	high	medium
C-2	medium	medium	low	medium	medium
C-3	low	low	high	medium	high

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.3, 0.4, 0.5	0.4, 0.5, 0.6	0.2, 0.3, 0.4	0.7, 0.8, 0.9	0.3, 0.4, 0.5
pos-SPIONs	0.4, 0.5, 0.6	0.4, 0.5, 0.6	0.1, 0.2, 0.3	0.4, 0.5, 0.6	0.3, 0.4, 0.5
neg-SPIONs	0.2, 0.3, 0.4	0.1, 0.2, 0.3	0.7, 0.8, 0.9	0.4, 0.5, 0.6	0.6, 0.7, 0.8

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.4	0.5	0.3	0.8	0.4
pos-SPIONs	0.5	0.5	0.2	0.5	0.4
neg-SPIONs	0.3	0.2	0.8	0.5	0.7

2. Determine the weights of alternatives for each criterion.

Table 2 shows the weight of alternatives for each criterion.

As the sums of weight values were more than 1.0, they were normalized in the TOPSIS code used for this analysis.

3. Determine the values in the criteria matrix.

The next step is obtaining the data of the criteria matrix.

Table 2 – The weights of alternatives for criteria

Alternatives /Values	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
C1-C3	0.5	0.5	0.5	0.5	0.5

Table 3 shows the criteria matrix in which the words "True" and "false" indicate the profit and cost criteria, respectively. In this matrix, antibiofilm activity, hemocompatibility, activity with hydrogen peroxide and rheological properties are profit criteria for SPIONs, whereas labour of their chemical synthesis is a cost criterion for these nanoparticles, respectively.

Table 3 – Criteria matrix

Alternatives /Values	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
C1-C3	True	True	True	True	False

4. Normalization step for fuzzy membership degrees and weights.

The results of the vector normalization performed on the fuzzy membership degrees of the characteristics of SPIONs as well as those of the normalization carried out on their weights, are represented in Tables 4 and 5, respectively.

Table 4 – The normalized decision matrix

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.565685	0.680414	0.341882	0.749269	0.444444
pos-SPIONs	0.707107	0.680414	0.227921	0.468293	0.444444
neg-SPIONs	0.424264	0.272166	0.911685	0.468293	0.777778

Table 5 – The weighted normalized decision matrix

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.113137	0.136083	0.068376	0.149854	0.088889
pos-SPIONs	0.141421	0.136083	0.045584	0.093659	0.088889
neg-SPIONs	0.084853	0.054433	0.182337	0.093659	0.155556

5. Determine the values of the best alternative and the worst alternative.

Table 6 shows the values of the best alternative and the worst alternative.

6. Determine the distances from the alternatives.

Table 7 shows the values of the distances from the best and the worst alternatives represented with (d_i^*) and (d_i^-), respectively.

Table 6 – The best alternative (A^+) and the worst alternative (A^-)

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
A^+	0.141421	0.136083	0.182337	0.149854	0.088889
A^-	0.084853	0.054433	0.045584	0.093659	0.155556

7. Determine the values of the similarity coefficients.

Table 8 shows the similarity coefficients (CC_i) and the rankings of the candidates according to their worst similarity.

Table 7 – The distances between the best and the worst alternatives

Candidates	d_i^*	d_i^-
neutral SPIONs	0.117418	0.124854
pos-SPIONs	0.147849	0.119629
neg-SPIONs	0.132170	0.136753

The improvement of the activity of positively charged SPIONs with hydrogen peroxide can increase to 0.3. In this case, we obtain a better ranking for these nanoparticles than those of the same nanoparticles in the first analysis series.

Table 8 – The similarity coefficients and the ranking of the candidates

Candidates	CC_i	ranking
neutral SPIONs	0.515346	1
pos-SPIONs	0.447249	3
neg-SPIONs	0.508520	2

The improvement of the activity of positively charged SPIONs with hydrogen peroxide can increase to 0.3. In this case, we obtain a better ranking for these nanoparticles than those of the same nanoparticles in the first analysis series. Tables 9 and 10 show the mean values of triangular fuzzy membership degrees of the characteristics of SPIONs and the results obtained with TOPSIS following this modification.

The only difference in the data of tables 9 and 1 concerns the mean value of the triangular fuzzy membership degree of the activity of positively charged SPIONs changed from 0.2 to 0.3.

Table 9 – The mean values of triangular fuzzy membership degrees of the characteristics of SPIONs

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.4	0.5	0.3	0.8	0.4
pos-SPIONs	0.5	0.5	0.3	0.5	0.4
neg-SPIONs	0.3	0.2	0.8	0.5	0.7

The weights of each alternative for each criterion and the values in the criteria matrix were used in this second series of analyses as presented in Tables 2 and 3.

Tables 11, 12, and 13 show the weighted normalized decision matrix, the best alternative (A^+) and the worst alternative (A^-), and the distances from the best alternative (d_i^*) and the worst alternative (d_i^-) for the candidates, respectively.

Table 10 – The normalized decision matrix

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.565685	0.680414	0.331295	0.749269	0.444444
pos-SPIONs	0.707107	0.680414	0.331295	0.468293	0.444444
neg-SPIONs	0.424264	0.272166	0.883452	0.468293	0.777778

Table 11 – The weighted normalized decision matrix

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.113137	0.136083	0.066259	0.149855	0.088889
pos-SPIONs	0.141421	0.136083	0.066259	0.093659	0.088889
neg-SPIONs	0.084853	0.054433	0.176690	0.093659	0.093659

Table 12 – The best alternative (A^+) and the worst alternative (A^-)

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
A^+	0.141421	0.136083	0.176690	0.149854	0.088889
A^-	0.084853	0.054433	0.066259	0.093659	0.155556

Table 13 – The distances from the best alternative and the worst alternative for candidates

Candidates	d_i^*	d_i^-
neutral SPIONs	0.113996	0.122756
pos-SPIONs	0.123907	0.119629
neg-SPIONs	0.132170	0.110432

Table 14 – The similarity coefficients and the ranking of the candidates

Candidates	CC_i	ranking
neutral SPIONs	0.518500	1
pos-SPIONs	0.491216	2
neg-SPIONs	0.455196	3

The comparison of Tables 8 and 14 shows that the ranking of SPIONs is affected after the change in the mean value of triangular fuzzy membership degree of the reactivity of positively charged SPIONs with hydrogen peroxide from 0.2 to 0.3. In the first ranking before this modification, these nanoparticles were ranked in the third place, whereas they appeared in the second place after this modification.

Fuzzy logic is a non-classical logic with applications in sciences and engineering [55–59]. A prediction model called the model of the tree has been applied for the improvement of these applications [60]. This model can be used to determine the number of profit and cost criteria and predict the impact of inappropriate consideration of the nanoparticles' characteristics on their ranks. The application of fuzzy logic in this model was explained previously [60]. The fuzzy logic disjunction operator is an important operator in this logic that can determine the effect of the simultaneous consideration of entities. Lukasiewicz's type disjunction can be used in fuzzy matrices [61, 62].

In another analysis series, Lukasiewicz's type disjunction was used to determine the impact of the simultaneous consideration of the labour for the chemical synthesis of SPIONs. This analysis was aimed to determine the effect of the inappropriate consideration and underestimation of this criterion for these nanoparticles. Suppose the manufacturer who synthesizes these nanoparticles while comparing with other nanoparticles considers that the labour for the preparation of neutral SPIONs and positively charged SPIONs is not high. In that case, the confusion in consideration of their manufacturing procedure due to the confusion of categories and inconsistency in his epistemic beliefs on their characteristics can change the ranks of these nanoparticles. If the membership degrees for the labor required for the preparation of other nanoparticles are as high as 0.6 or more, the summation of the fuzzy degree memberships of this criterion for these two types of SPIONs and those of other nanoparticles would be 1.0 or greater than 1.0. The maximal value of Lukasiewicz's type disjunction is 1.0. So, the value of 1.0 will appear as the maximum value in the output of TOPSIS.

Tables 15 and 16 show the mean values of the triangular fuzzy membership degrees of the characteristics of SPIONs and the output of modified TOPSIS after their consideration with other nanoparticles.

Table 15 – The mean values of triangular fuzzy membership degrees of the characteristics of SPIONs after consideration with other nanoparticles

Candidates/ criteria	antibiofilm activity	hemocompatibility	activity with hydrogen peroxide	rheological properties	labour of their chemical synthesis
neutral SPIONs	0.4	0.5	0.3	0.8	1.0
pos-SPIONs	0.5	0.5	0.2	0.5	1.0
neg-SPIONs	0.3	0.2	0.8	0.5	0.7

Table 16 – The similarity coefficients and the ranking of the candidates according to the worst similarity

Candidates	CC_i	ranking
neutral SPIONs	0.461011	3
pos-SPIONs	0.394185	1
neg-SPIONs	0.554313	2

As shown in Table 16, the positively charged SPIONs and negatively charged SPIONs are ranked in the first and second positions, respectively, whereas the neutral SPIONs are ranked in the third position. This is due to Lukasiewicz's type disjunction in the TOPSIS code and the summation of the degrees of membership of SPIONs and other nanoparticles.

As TOPSIS has been used to optimize manufacturing processes [63–66], the modification of this algorithm with the fuzzy disjunction operator, as explained in this work can help investigate the impact of the confusion of categories when the criteria for the manufacture of materials are selected. Fuzzy logic also has other operators such as conjunction operator and implication operator. These operators can also be implemented in the TOPSIS code to determine the other situations affecting the manufacturing processes [67–73].

Other non-classical logic, such as modal logic and computability logic [74], can also be used in the TOPSIS analysis, including the issues explained in this paper for the optimization of nanoparticle manufacture.

In recent years, several nanomaterials and biomaterials' physicochemical and biological properties have been investigated [75–80]. These works have revealed the properties and activities of these materials for their manufacture as well as their applications in diverse fields of science and engineering [81–85]. Further investigations are required for the analysis of the properties of these materials with TOPSIS.

4 Conclusions

The properties of nanoparticles are diverse and require being ranked to determine which of these nanoparticles has the best characteristics in comaprison with the others. This paper presents the characteristics of SPIONs, and their impact on ranking these nanoparticles has been explained. The results obtained in this study show that neutral SPIONs have a better rank of positively charged and negatively charged nanoparticles. Moreover, improving the activity of positively charged SPIONs with hydrogen peroxide can affect their rank. These results are promising for the manufacture of the next generations of SPIONs. Moreover, they can be helpful in a comparative study of these nanoparticles with the other ones. The results can be applied in the comparative optimization of the manufacturing procedures of these nanoparticles.

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