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OPTIMIZATION OF CHEMICAL SYNTHESIS OUTPUT WITH TOPSIS

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Abstract. The present study focuses on a new application of a decision-making process using the Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) method for the optimization of the chemical synthesis output. This investigation is important as many chemical reactions have been performed in labs without any analysis of their optimization. The factors that affect the chemical synthesis output such as catalyst, nanosensor network, and temperature have been considered in this study. Moreover, labor that corresponds to the prices of chemicals that are used in chemical reactions has also been considered. Different chemical synthesis procedures with or without these factors have been analyzed in the current study. In the first series of analyses, the same weight values were considered for all criteria, whereas in the second series of analyses, the weight values for the nanosensor network and labor were more than those of catalyst and temperature. The obtained results showed that the consideration of profit criteria and cost criteria and equal or different weights for the candidates could affect the output of TOPSIS. Therefore, the prediction of the chemical synthesis output using this algorithm for three different conditions for performing chemical reactions. Moreover, it was shown that different considerations of these conditions could help optimize the reactions. In the first series of analysis, the second candidate was ranked in the first position, whereas the third candidate and the first candidates were positioned in the second and third positions, respectively. The ranking of candidates was different in the second series of analysis as the first, second, and third candidates were ranked in the first, second, and third positions, respectively. The results of this investigation can be used for the optimization of chemical reactions and lab procedures.

Key words: Optimization; Prediction; Chemical synthesis; Decision-making procedure; TOPSIS.

Introduction

Chemical synthesis is an important procedure that is used in labs for the preparation or modification of materials [1], [2]. In this procedure, different chemical reactions are used in which their output is affected by factors such as a catalyst [3], nanosensor network [4], or temperature [5].

The Development of appropriate methods enabling the synthesis of important molecules in reasonable yields, the performance of with the selectivities typical of enzymatic reactions, the exploration of important properties in synthetic materials, the design of synthetic procedures to optimize the properties of products, the synthesis of new substances with self-assemble into complex organized systems, and the use of catalysts in the synthesis and manufacture of materials are among the challenges for performing appropriate chemical reactions [6], [7].

Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) is a method that has been largely used for the prediction and optimization of materials [8], [9], [10], [11]. The applications of TOPSIS have been diverse in science and engineering. However, this method has never been used previously for the optimization of the output of chemical synthesis. It has been shown that TOPSIS would be an efficient technique for the prediction and optimization of different issues such as behavior, methods,
materials and types of equipment [12], [13], [14], [15], [16] as well as its further application for the optimization of the composites has also been investigated [17], [18], [19].

In this study, the factors that affect the output of chemical syntheses such as catalyst, nanosensor network, and temperature have been considered. Moreover, the labor for performing the chemical synthesis has also been considered in this investigation.

The objective of the current work was to determine which one of these factors could have more effect of the ranks of candidates. Moreover, it was aimed to optimize the chemical synthesis according to the ranking obtained in the first series of analyses. For this purpose, a second series of analyses with different weight values was performed with TOPSIS.

The paper is organized as follows: Section 2 presents the research methodology including the information on the selection of candidates and TOPSIS. Section 3 presents the results and discussion and section 4 includes the conclusions derived from the obtained results.

The results of this investigation can be used for the optimization of different chemical synthesis procedures in science and engineering.

**Experimental approach**

*Selection of candidates*

The chemical reactions were the candidates, which were selected according to the synthesis output. $C_1$, $C_2$ and $C_3$ indicate the candidates with outputs that were affected differently with the addition of a catalyst, nanosensor network, and increase in temperature, respectively.

**TOPSIS method**

The TOPSIS software in Python used in this study was described previously [10]. The data in the evaluation matrix, the weight matrix, and the criteria matrix were entered into the software. Then, the distances from the best and worst alternatives as well as the closeness coefficients were determined for each chemical reaction according to the formulas explained in the previous work [10].

**Results and discussion**

Table 1 shows the terms and mean values of fuzzy membership degrees of the characteristics of the chemical reactions.

<table>
<thead>
<tr>
<th>Candidates/ Criteria</th>
<th>Catalyst</th>
<th>Nano sensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
</tr>
<tr>
<td>$C_2$</td>
<td>Medium</td>
<td>Low</td>
<td>Medium</td>
<td>Medium</td>
</tr>
<tr>
<td>$C_3$</td>
<td>Medium</td>
<td>Low</td>
<td>High</td>
<td>Medium</td>
</tr>
</tbody>
</table>

Table 2 shows the weights of alternatives for each candidate’s characteristics.

<table>
<thead>
<tr>
<th>Alternatives / values</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$-$C_3$</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 3 shows the criteria matrix in which the terms “true” and “false” were chosen for the profit criteria and cost criterion, respectively.

<table>
<thead>
<tr>
<th>Alternatives/values</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$-$C_3$</td>
<td>True</td>
<td>True</td>
<td>True</td>
<td>False</td>
</tr>
</tbody>
</table>
Optimization of physical instruments’ characteristics with TOPSIS

Tables 4 and 5 show the data in the normalized decision matrix and weighted normalized decision matrix, respectively.

**Table 4**

<table>
<thead>
<tr>
<th>Candidates/Criteria</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.27216553</td>
<td>0.57735027</td>
<td>0.20739034</td>
<td>0.20739034</td>
</tr>
<tr>
<td>C₂</td>
<td>0.68041382</td>
<td>0.57735027</td>
<td>0.51847585</td>
<td>0.51847585</td>
</tr>
<tr>
<td>C₃</td>
<td>0.68041382</td>
<td>0.57735027</td>
<td>0.82956136</td>
<td>0.82956136</td>
</tr>
</tbody>
</table>

**Table 5**

<table>
<thead>
<tr>
<th>Candidates/Criteria</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.06804138</td>
<td>0.14433757</td>
<td>0.05184758</td>
<td>0.05184758</td>
</tr>
<tr>
<td>C₂</td>
<td>0.17010345</td>
<td>0.14433757</td>
<td>0.12961896</td>
<td>0.12961896</td>
</tr>
<tr>
<td>C₃</td>
<td>0.17010345</td>
<td>0.14433757</td>
<td>0.20739034</td>
<td>0.20739034</td>
</tr>
</tbody>
</table>

Table 6 shows the results of the best alternative and the worst alternative for the candidates.

**Table 6**

<table>
<thead>
<tr>
<th>Candidates/Criteria</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.17010345</td>
<td>0.14433757</td>
<td>0.20739034</td>
<td>0.05184758</td>
</tr>
<tr>
<td>A</td>
<td>0.06804138</td>
<td>0.14433757</td>
<td>0.05184758</td>
<td>0.20739034</td>
</tr>
</tbody>
</table>

Table 7 shows the results of the distances from the best and the worst alternatives for the candidates.

**Table 7**

<table>
<thead>
<tr>
<th>Candidates</th>
<th>$D_i^+$</th>
<th>$D_i^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.18603821</td>
<td>0.15554275</td>
</tr>
<tr>
<td>C₂</td>
<td>0.10998534</td>
<td>0.1500448</td>
</tr>
<tr>
<td>C₃</td>
<td>0.15554275</td>
<td>0.18603821</td>
</tr>
</tbody>
</table>

Table 8 shows the similarity coefficients and the rankings of the chemical reactions that have been obtained according to their worst similarity.

**Table 8**

<table>
<thead>
<tr>
<th>Candidates</th>
<th>$CC_i$</th>
<th>Ranking</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.45536131</td>
<td>2</td>
</tr>
<tr>
<td>C₂</td>
<td>0.5770285</td>
<td>3</td>
</tr>
<tr>
<td>C₃</td>
<td>0.54463869</td>
<td>1</td>
</tr>
</tbody>
</table>

In another analysis, we investigated the effect of weights on the ranking of candidates. Higher weight values were considered for nanosensor network and labor in comparison with those of the first series of analysis.
Table 9 shows the mean values of fuzzy membership degrees of the characteristics of candidates.

<table>
<thead>
<tr>
<th>Candidates/ Criteria</th>
<th>Catalyst</th>
<th>Nano sensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>C₂</td>
<td>0.5</td>
<td>0.2</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>C₃</td>
<td>0.5</td>
<td>0.2</td>
<td>0.8</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Table 10 shows the weights of alternatives for each candidate’s characteristics.

<table>
<thead>
<tr>
<th>Alternatives/values</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁–C₃</td>
<td>0.5</td>
<td>0.8</td>
<td>0.5</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Table 11 shows the criteria matrix in which the terms “true” and “false” were chosen for the profit criteria and cost criterion, respectively.

<table>
<thead>
<tr>
<th>Alternatives/values</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁–C₃</td>
<td>True</td>
<td>True</td>
<td>True</td>
<td>False</td>
</tr>
</tbody>
</table>

Table 12 shows the results obtained in the normalized decision matrix.

<table>
<thead>
<tr>
<th>Candidates / Criteria</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.27216553</td>
<td>0.57735027</td>
<td>0.20739034</td>
<td>0.20739034</td>
</tr>
<tr>
<td>C₂</td>
<td>0.68041382</td>
<td>0.57735027</td>
<td>0.51847585</td>
<td>0.51847585</td>
</tr>
<tr>
<td>C₃</td>
<td>0.68041382</td>
<td>0.57735027</td>
<td>0.82956136</td>
<td>0.82956136</td>
</tr>
</tbody>
</table>

Table 13 shows the results obtained in the weighted normalized decision matrix.

<table>
<thead>
<tr>
<th>Candidates/ Criteria</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.05233952</td>
<td>0.17764624</td>
<td>0.03988276</td>
<td>0.06381241</td>
</tr>
<tr>
<td>C₂</td>
<td>0.13084881</td>
<td>0.17764624</td>
<td>0.09970689</td>
<td>0.15953103</td>
</tr>
<tr>
<td>C₃</td>
<td>0.13084881</td>
<td>0.17764624</td>
<td>0.15953103</td>
<td>0.25524965</td>
</tr>
</tbody>
</table>
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Table 14 shows the results of the best alternative (A⁺) and the worst alternative (A⁻).

<table>
<thead>
<tr>
<th>Candidates/ Criteria</th>
<th>Catalyst</th>
<th>Nanosensor network</th>
<th>Temperature</th>
<th>Labor</th>
</tr>
</thead>
<tbody>
<tr>
<td>A⁺</td>
<td>0.13084881</td>
<td>0.17764624</td>
<td>0.15953103</td>
<td>0.06381241</td>
</tr>
<tr>
<td>A⁻</td>
<td>0.05233952</td>
<td>0.17764624</td>
<td>0.03988276</td>
<td>0.25524965</td>
</tr>
</tbody>
</table>

Table 15 shows the results of distances from the best alternative (d⁺) and the worst alternative (d⁻) for the candidates.

<table>
<thead>
<tr>
<th>Candidates</th>
<th>d⁺</th>
<th>d⁻</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.14310631</td>
<td>0.19143724</td>
</tr>
<tr>
<td>C₂</td>
<td>0.11287595</td>
<td>0.13749432</td>
</tr>
<tr>
<td>C₃</td>
<td>0.19143724</td>
<td>0.14310631</td>
</tr>
</tbody>
</table>

Table 16 shows the similarity coefficients (CCᵢ) and the ranking of the candidates.

<table>
<thead>
<tr>
<th>Candidates</th>
<th>CCᵢ</th>
<th>Ranking</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.57223413</td>
<td>1</td>
</tr>
<tr>
<td>C₂</td>
<td>0.54916392</td>
<td>2</td>
</tr>
<tr>
<td>C₃</td>
<td>0.42776587</td>
<td>3</td>
</tr>
</tbody>
</table>

The results of this paper showed that TOPSIS could be used for the optimization of the chemical synthesis output. As shown in two different series of analyses, the prediction of the chemical synthesis output was performed with this algorithm for three different conditions. It was also shown that different considerations of these conditions could help get an appropriate optimization of the chemical reactions.

The physical, chemical, and biological properties of some (nano)materials have been investigated in recent years [20], [21], [22], [23], [24]. Moreover, some previous studies have been focused on the characterization of different devices and materials [25], [26], [27], [28], [29]. These properties could be predicted and optimized with TOPSIS. Some other optimization methods such as genetic algorithm, bidirectional evolutionary structure optimization, and Bayesian optimization have been used for the characteristic optimization of materials [30], [31], [32], [33], [34]. It has been shown that machine learning models would be capable of predicting the properties of materials [35], [36], [37], [38]. However, the applicants of these models are faced with some issues and challenges such as data preparation and cleaning, high dimension problems, adjustable parameters, etc. [39], [40], [41], [42], [43]. More investigations would be required for the optimization of tuned materials with these methods for the output improvement of chemical reactions.

Conclusions

This paper presented the optimization of chemical reactions considering catalysts, nanosensor networks, and temperature that affect their outputs. Two series of analyses were performed to determine which factor was dominant in the ranking of candidates and which modification could improve the ranks. The same weight values were considered for all criteria in the first series of analyses. In the second series
of analyses, the weight values of the nanosensor network and labor as two factors affecting the output of chemical synthesis were increased. It was shown that the ranks of candidates would change with this modification. The first candidate that was ranked in the third position in the first series of analyses was ranked in the first position in the second series of analyses. The second and third candidates having the first and second ranks in the first series of analyses had the second and third ranks in the second series of analyses, respectively.

References


