UKRAINIAN JOURNAL OF MECHANICAL ENGINEERING AND MATERIALS SCIENCE
Vol. 10, No. 1, 2024

Taraneh Javanbakht[1, 2]

[1] Department of Chemistry and Biochemistry, Department of Physics, Concordia University, Richard J. Renaud Science Complex, 7141, Sherbrooke str. West, Montreal, Quebec, Canada H4B 1R6
[2] Department of Computer Science, University of Quebec in Montreal, 201, President Kennedy str., Montreal, Quebec, Canada H2X 3Y7

E-mail: javanbakht.taraneh@courrier.uqam.ca, ORCID 0000-0002-2658-330X

OPTIMIZATION OF CHEMICAL SYNTHESIS OUTPUT WITH TOPSIS

Received: December 15, 2023 / Revised: December 28, 2023 / Accepted: January 9, 2024

https://doi.org/10.23939/ujmems2024.01.063

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 1

The Terms and mean values of fuzzy membership degrees of the characteristics of chemical reactions

Candidates/ Criteria	Catalyst	Nano sensor network	Temperature	Labor
C_1	Low	Low	Low	Low
C_2	Medium	Low	Medium	Medium
C_3	Medium	Low	High	High

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

Table 2

Weights of alternatives for each candidate's characteristic

Alternatives / values	Catalyst	Nanosensor network	Temperature	Labor
C_1-c_3	0.5	0.5	0.5	0.5

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

Table 3

Criteria matrix for chemical reactions

Alternatives/values	Catalyst	Nanosensor network	Temperature	Labor
C1-c3	True	True	True	False

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

Table 4

The normalized decision matrix for chemical reactions

Candidates/ Criteria	Catalyst	Nanosensor network	Temperature	Labor
C_1	0.27216553	0.57735027	0.20739034	0.20739034
C_2	0.68041382	0.57735027	0.51847585	0.51847585
C_3	0.68041382	0.57735027	0.82956136	0.82956136

Table 5

The weighted normalized decision matrix for chemical reactions

Candidates/ Criteria	Catalyst	Nanosensor network	Temperature	Labor
C_1	0.06804138	0.14433757	0.05184758	0.05184758
C_2	0.17010345	0.14433757	0.12961896	0.12961896
C_3	0.17010345	0.14433757	0.20739034	0.20739034

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

Table 6

The best alternative and the worst alternative for chemical reactions

Candidates/ Criteria	Catalyst	Nano sensor network	Temperature	Labor
A^+	0.17010345	0.14433757	0.20739034	0.05184758
A^-	0.06804138	0.14433757	0.05184758	0.20739034

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

Table 7

The ***distances from the best and the worst alternatives for chemical reactions***

Candidates	D_i^*	D_i^-
C_1	0.18603821	0.15554275
C_2	0.10998534	0.1500448
C_3	0.15554275	0.18603821

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

Table 8

Similarity coefficients and rankings of chemical reactions

Candidates	CC_i	Ranking
C_1	0.45536131	2
C_2	0.5770285	3
C_3	0.54463869	1

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 9

The fuzzy membership degrees of the characteristics of chemical reactions

Candidates/ Criteria	Catalyst	Nano sensor network	Temperature	Labor
C_1	0.2	0.2	0.2	0.2
C_2	0.5	0.2	0.5	0.5
C_3	0.5	0.2	0.8	0.8

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

Table 10

Weight factors of alternatives for each candidate's characteristic

Alternatives/values	Catalyst	Nanosensor network	Temperature	Labor
C_1–C_3	0.5	0.8	0.5	0.8

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

Table 11

Criteria matrix for chemical reactions

Alternatives/values	Catalyst	Nanosensor network	Temperature	Labor
C_1–C_3	True	True	True	False

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

Table 12

The normalized decision matrix for chemical reactions

Candidates / Criteria	Catalyst	Nanosensor network	Temperature	Labor
C_1	0.27216553	0.57735027	0.20739034	0.20739034
C_2	0.68041382	0.57735027	0.51847585	0.51847585
C_3	0.68041382	0.57735027	0.82956136	0.82956136

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

Table 13

The weighted normalized decision matrix for chemical reactions

Candidates/ Criteria	Catalyst	Nanosensor network	Temperature	Labor
C_1	0.05233952	0.17764624	0.03988276	0.06381241
C_2	0.13084881	0.17764624	0.09970689	0.15953103
C_3	0.13084881	0.17764624	0.15953103	0.25524965

Table 14 shows the results of the best alternative (A^+) and the worst alternative (A^-).

Table 14

The best alternative and the worst alternative for chemical reactions

Candidates/ Criteria	Catalyst	Nanosensor network	Temperature	Labor
A^+	0.13084881	0.17764624	0.15953103	0.06381241
A^-	0.05233952	0.17764624	0.03988276	0.25524965

Table 15 shows the results of distances from the best alternative (d_i^*) and the worst alternative (d_i^-) for the candidates.

Table 15

The distances from the best and the worst alternatives for chemical reactions

Candidates	d_i^*	d_i^-
C_1	0.14310631	0.19143724
C_2	0.11287595	0.13749432
C_3	0.19143724	0.14310631

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

Table 16

Similarity coefficients and rankings of chemical reactions

Candidates	CC_i	Ranking
C_1	0.57223413	1
C_2	0.54916392	2
C_3	0.42776587	3

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

[1] Bartlewicz, O. et al. Heterogeneous catalysis with the participation of ionic liquids, *Catalysts*, 10(11), 1227, 2020. https://doi.org/10.3390/catal10111227.

[2] Chen, W. et al. Mesoporous cobalt-iron-organic frameworks: plasma-enhanced oxygen evolution electrocatalyst, *Journal of Materials Chemistry A*, 7(7), 2019. https://doi.org/10.1039/C8TA10952D.

[3] Vogiatzis, K. D. et al. Computational approach to molecular catalysis by 3d transition metals: Challenges and opportunities, 119, 4, 2453–2523, 2019. https://doi.org/10.1021/acs.chemrev.8b00361.

[4] Zarepour, E. et al. Nano sensor networks for tailored operation of highly efficient gas-to-liquid fuels catalysts, The University of New South Wales, *Technical Report,* UNSW-CSE-TR-201318, 2013.

[5] Chodosh, D. F. et al. Automated chemical synthesis. Part 3: Temperature control systems, *Journal of Automatic Chemistry*, 5(2), 103–107, 1983.

[6] Synthesis and manufacturing: Creating and exploiting new substances and new transformations in *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering*, Washington: National Academies Press (US); 2003.

[7] Levin, I. et al. Merging enzymatic and synthetic chemistry with computational synthesis planning, *Nature Communications*, 13, 7747, 2022. https://doi.org/10.1038/s41467-022-35422-y.

[8] Huang, W. F. An improved TOPSIS method for material selection model, *Advanced Materials Research*, 951, 120–123, 2014. https://doi.org/10.4028/www.scientific.net/AMR.951.120.

[9] Ma, F. et al. A comprehensive MCDM model combining TOPSIS and IEM for sustainable material selection considering life cycle assessment method, *IEEE Access*, 99, 1–1, 2018. https://doi.org/10.1109/ACCESS.2018.2875038.

[10] Javanbakht, T. Optimization of Cdx transcription factors characteristics, *Journal of Engineering Sciences*, 10(2), E1-E7, 2023. https://doi.org/10.21272/jes.2023.10(2).e1.

[11] Zakeri, S. et al. A decision analysis model for material selection using simple ranking process, *Scientific Reports*, 8631, 2023. https://doi.org/10.1038/s41598-023-35405-z.

[12] Javanbakht, T., Chakravorty, S. Prediction of human behavior with TOPSIS, *Journal of Fuzzy Extension and Applications*, 3 (2), 109–125, 2022.

[13] Javanbakht, T., Chakravorty, S. Optimization of machine learning algorithms for proteomic analysis using topsis, *Journal of Engineering Sciences*, 9 (2), E7-E12, 2022.

[14] Amrabadi, T. et al. Application of TOPSIS algorithm in describing bacterial cellulose-based composite hydrogel performance in incorporating methylene blue as a model drug, *Scientific Reports*, 13, 2755, 2023.

[15] Javanbakht, T. Analysis of nanoparticles characteristics with TOPSIS for their manufacture optimization, *Journal of Engineering Sciences*, 9 (2), C1–C8, 2022.

[16] Javanbakht, T. Optimization of physical instruments' characteristics with TOPSIS, *Ukrainian Journal of Mechanical Engineering and Materials Science*, 8 (3), 1-9, 2022.

[17] Jha, K. et al. Application of modified TOPSIS technique in deciding optimal combination for bio-degradable composite, *Vacuum*, 157, 259–267, 2018.

[18] Sanjay, M. R. et al. TOPSIS method for selection of best composite laminate, in *Modelling of Damage Processes in Biocomposites, Fibre-Reinforced Composites and Hybrid Composites*, Woodhead Publishing Series in Composites Science and Engineering, 199–209, 2019.

[19] Dukkipati, B. N. et al. TOPSIS ranking of epoxy hybrid composites, *IJESC*, 15244, 2017.

[20] Javanbakht, T., Laurent, S., Stanicki, D., Frenette, M. (2020). Correlation between physicochemical properties of superparamagnetic iron oxide nanoparticles and their reactivity with hydrogen peroxide, *Canadian Journal of Chemistry*, Vol. 98(10), pp. 601–608. https://doi.org/10.1139/cjc-2020-0087.

[21] Javanbakht, T., Laurent, S., Stanicki, D., David, E. Related physicochemical, rheological, and dielectric properties of nanocomposites of superparamagnetic iron oxide nanoparticles with polyethyleneglycol, *Journal of Applied Polymer Science*, 136:48280–48290, 2019. https://doi.org/10.1002/app.48280.

[22] Javanbakht, T., Sokolowski, W. Thiol-ene/acrylate systems for biomedical shape-memory polymers, *Shape Memory Polymers for Biomedical Applications*, 157–166, 2015. https://doi.org/10.1016/B978-0-85709-698-2.00008-8.

[23] Javanbakht, T., Hadian, H., Wilkinson, K. J. Comparative study of physicochemical properties and antibiofilm activity of graphene oxide nanoribbons, *Journal of Engineering Sciences*, 7(1):C1–C8, 2020. https://doi.org/10.21272/jes.2020.7(1).c1.

[24] Soares, S. et al. Nanomedicine: Principles, properties, and regulatory issues, *Frontiers*, 6, 2018.

[25] Singh, J. *Electronic and optoelectronic properties of semiconductor structures*, Cambridge University Press, 2003.

[26] Javanbakht, T., Ghane-Motlagh, B., Sawan, M. Comparative study of antibiofilm activity and physicochemical properties of microelectrode arrays, *Microelectronic Engineering*, 229:111305, 2020. https://doi.org/10.1016/j.mee.2020.111305.

[27] Javanbakht, T., David, E. Rheological and physical properties of a nanocomposite of graphene oxide nanoribbons with polyvinyl alcohol, *Journal of Thermoplastic Composite Materials*, 0892705720912767, 2020. https://doi.org/10.1177/0892705720912767.

[28] Murugan, S.S. Mechanical properties of materials: Definition, testing and application, *International Journal of Modern Studies in Mechanical Engineering*, 6, 2, 28–38, 2020.

[29] Djavanbakht, T., Carrier, V., André, J. M., Barchewitz, R, Troussel, P. Effets d'un chauffage thermique sur les performances de miroirs multicouches Mo/Si, Mo/C et Ni/C pour le rayonnement X mou, *Journal de Physique IV*, France, 10:281–287, 2000. https://doi.org/10.1051/jp4:20001031.

[30] Nagadeepan, A. et al. Advanced optimization of surface characteristics and material removal rate for biocompatible Ti6Al4V using WEDM process with BBD and NSGA II, *Materials*, 16(14), 4915, 2023.

[31] Wierzbanowski, K. et al. Optimization of material properties using genetic algorithms, *Materials Science Forum*, 652, 1–6, 2010.

[32] Gan, N., Wang, Q. Topology optimization of multiphase materials with dynamic and static characteristics by BESO method, *Advances in Engineering Software*, 151, 102928, 2021.

[33] Zhang, Y. et al. Bayesian optimization for materials design with mixed quantitative and qualitative variables, *Scientific Reports*, 4924, 2020.

[34] Deshwal, A. et al. Bayesian optimization of nanoporous materials, *Molecular Systems Design and Engineering*, 6, 12, 1066–1086, 2021.

[35] Allen, A. A., Tkatchenko, A. Machine learning of material properties: Predictive and interpretable multilinear models, *Science Advances*, 8, 18, 2022.

[36] Tian, X.-L. et al. Machine learning-guided property prediction of energetic materials: Recent advances, challenges, and perspectives, *Energetic Materials Frontiers*, 3, 3, 177–186, 2022.

[37] Ward, L. et al. A general-purpose machine learning framework for predicting properties of inorganic materials, *Computational Materials*, 16028, 2016.

[38] Chibani, S., Coudert, F.-X. Machine learning approaches for the prediction of materials properties, *APL Materials*, 8(8), 080701, 2020.

[39] Vasicek, D. Artificial intelligence and machine learning: Practical aspects of overfitting and regularization, Information Services and Use, 39(4), 1–9, 2019.

[40] Ohlsson, C. *Exploring the potential of machine learning*, Thesis, 2017.

[41] Kim, P. *MATLAB deep learning: With machine learning, neural networks and artificial intelligence*, Apress, 2017.

[42] Morgan, D., Jacobs, R. Opportunities and challenges for machine learning in materials science, *Annual Review of Materials Research*, 50, 71–103, 2020.

[43] Haykin, S. *Neural networks and learning machines*, Prentice Hall, 2009.