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Application Of TOPSIS For Optimal Solvent Selection In The Oxidation Of Tryptophan By Chromium Complexes

[1]Ammilal Rao, [2]Gaurav Sharma, [3]Ganesh Kumar
[1]Assistan Professor, [2]Associate Professor, [3]Asistant Professor
[1]Departemt of Chemistry,
[1]University of Rajasthan, Jaipur, India
[2]Departemt of Mathematics, Acharya Narendra Dev College,
[2]University of Delhi, Delhi, India
[3]Departemt of Mathematics,
[3]University of Rajasthan, Jaipur, India

Abstract: The selection of an appropriate solvent plays a crucial role in determining the efficiency of oxidation reactions, particularly in the case of bio-molecules like tryptophan. This study presents a Multi-Criteria Decision-Making (MCDM) approach using the TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) method to evaluate and rank five solvents—Chloroform (CF), Dichloroethane (DCE), Dichloromethane (DCM), Dimethyl sulfoxide (DMSO), and Dimethylformamide (DMF)—based on five performance parameters: Initial Decomposition Constant (IDC), Quenching Fluorescence Constant (QFC), Maximum Fluorescence Constant (MFC), Binding Percentage of Chromium Complex (BPCC), and Binding Tendency of Electron Accepting Chromium Complex (BTEACC). The decision matrix was normalized, weighted equally, and analyzed to determine the ideal and negative-ideal solutions. The results indicate that DMSO exhibits the highest closeness coefficient, emerging as the most suitable solvent for the oxidation of tryptophan by chromium complexes, followed by DMF. The findings provide a quantitative basis for solvent selection in coordination chemistry and oxidative bio-reactions.

***Keywords* -** TOPSIS, Multi-Criteria Decision Making (MCDM), Tryptophan Oxidation, Chromium Complexes, Solvent Selection.

1. INTRODUCTION

In the realm of multi-criteria decision-making (MCDM) and oxidation kinetics, extensive research has been conducted to explore theoretical models, experimental validation, and practical applications across diverse scientific and engineering domains.

Yeh (2003) explored the selection of appropriate multi-attribute decision-making methods for tasks such as scholarship selection. A significant method in this context is TOPSIS, which has undergone various developments as reviewed by Zavadskas et al. (2016), who provided a detailed overview of its evolution and widespread use in complex decision environments. To enhance its applicability, Kuo (2017) proposed a modified TOPSIS model using a different ranking index. Further advancements were made by Shyur and Shih (2006), who developed a hybrid MCDM framework for vendor selection, and by Ture et al. (2020), who applied integrated VIKOR and TOPSIS approaches for group strategy evaluations. Similarly, Tavana and Hatami-Marbini (2021) applied a group AHP-TOPSIS model to address strategic decision problems in NASA's spaceflight mission planning. TOPSIS has found practical applications in various modern decision problems. Khan et al. (2021) used MCDM techniques for drone selection, while Nanayakkara (2019) applied TOPSIS to guide students in choosing academic disciplines and universities. Akgül et al. (2021) demonstrated how TOPSIS could be utilized in textile engineering to design dyeing processes using natural colorants. Chedde et al. (2021) employed TOPSIS for the selection of materials in the design of powered hand trucks, and Laroche et al. (2005) evaluated service quality using empirical decision-making models. Applications have also extended to chemical decision contexts, as seen in the work of Soni et al. (2015) and U. Soni et al. (2015), where decision methods were used to analyze structure-reactivity relationships in the oxidation of benzaldehydes. Parallel to MCDM research, a substantial body of literature exists on the kinetics and mechanisms of oxidation reactions involving aliphatic aldehydes. Agarwal et al. (1990) studied the oxidation of aldehydes using pyridinium fluorochromate. Khanchandani et al. (1996) and Khurana et al. (1999) further examined the mechanisms of such oxidations using pyridinium bromochromate and quinolinium fluorochromate respectively. Kumbhat et al. (2000) explored oxidation reactions using bipyridinium chlorochromate, and Saraswat et al. (2001) contributed by detailing the kinetic behavior with pyridinium chlorochromate. Studies have expanded the range of reagents. Chouhan et al. (2006) investigated the oxidation of aldehydes with benzyltriethylammonium chlorochromate, while Kumbhat et al. (2007) focused on quinolinium bromochromate. Soni et al. (2008) evaluated morpholinium chlorochromate, and Patel et al. (2012) employed tetrakis(pyridine) silver dichromate (TPSD) as an oxidant in their kinetic studies. Daiya et al. (2012) analyzed structure-reactivity correlations in the oxidation of benzaldehydes with imidazolium fluorochromate, and Sharma et al. (2010) provided a kinetic and mechanistic study of similar reactions using the same oxidant. U. Soni et al. (2015) further contributed by analyzing reactivity patterns.

These studies form a rich foundation for understanding both the development of decision-making methodologies and the chemical kinetics of oxidation processes. The convergence of empirical kinetic data with structured decision-making models presents opportunities for enhanced analytical precision and optimization in scientific and industrial settings.

2.TOPSIS Method: Step-by-Step Procedure

TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) is a widely used multi-criteria decision-making (MCDM) method. It ranks alternatives based on their relative closeness to an ideal best and an ideal worst solution. Below is the step-by-step procedure.

Step 1: Construct the Decision Matrix
List all alternatives and criteria in a matrix form:

$$D = [x_{ij}]$$

Step 2: Normalize the Decision Matrix
Use vector normalization to eliminate scale differences:

$$r_{ij} = \frac{x_{ij}}{\sqrt{\sum_{i=1}^{m} x_{ij}^2}}$$

Step 3: Construct the Weighted Normalized Decision Matrix
Multiply each normalized value by its criterion weight:

$$v_{ij} = w_j \cdot r_{ij}$$

Step 4: Determine the Ideal Best (A^+) and Ideal Worst (A^-) Solutions

$$A^+ = \{\max(v_{ij}) \text{ if benefit, } \min(v_{ij}) \text{ if cost}\}$$
$$A^- = \{\min(v_{ij}) \text{ if benefit, } \max(v_{ij}) \text{ if cost}\}$$

Step 5: Calculate the Separation Measures
Calculate the distance from the ideal best and ideal worst:

$$S_i^+ = \sqrt{\sum_{j=1}^{n}(v_{ij} - A_j^+)^2} \quad \text{(Distance from ideal best)}$$

$$S_i^- = \sqrt{\sum_{j=1}^{n}(v_{ij} - A_j^-)^2} \quad \text{(Distance from ideal worst)}$$

Step 6: Calculate the Relative Closeness to the Ideal Solution

$$C_i = \frac{S_i^-}{S_i^+ + S_i^-}$$

, where $0 \leq C_i \leq 1$

Step 7: Rank the Alternatives
Rank alternatives in descending order of C_i. The higher the C_i, the better the alternative.

3. Step-by-Step Solution of the Model

Here are the complete tables for each step of the TOPSIS method:

Table-1: Decision Matrix

	IDC	**QFC**	**MFC**	**BPCC**	**BTEACC**
CF	24.9	8.80	25.0	10.9	22.7
DCE	20.7	7.50	22.7	8.80	19.8
DCM	23.7	8.20	23.2	12.1	20.6
DMSO	75.0	25.5	71.0	38.8	61.0
DMF	30.1	12.4	31.9	18.2	27.2

Table-2: Normalized Decision Matrix

	IDC	**QFC**	**MFC**	**BPCC**	**BTEACC**
CF	0.2760	0.2776	0.2842	0.2335	0.2983
DCE	0.2294	0.2366	0.2581	0.1885	0.2602
DCM	0.2627	0.2587	0.2638	0.2592	0.2707
DMSO	0.8312	0.8044	0.8072	0.8311	0.8015
DMF	0.3336	0.3912	0.3627	0.3899	0.3574

Table-3: Criteria Weights (Equal Weightage)

Criteria	IDC	QFC	MFC	BPCC	BTEACC
Weights	0.2	0.2	0.2	0.2	0.2

Table-4: Weighted Normalized Decision Matrix

Alternative	IDC	QFC	MFC	BPCC	BTEACC
CF	0.0552	0.0555	0.0568	0.0467	0.0597
DCE	0.0459	0.0473	0.0516	0.0377	0.0520
DCM	0.0525	0.0517	0.0528	0.0518	0.0541
DMSO	0.1662	0.1609	0.1614	0.1662	0.1603
DMF	0.0667	0.0782	0.0725	0.0780	0.0715

Table-5: Ideal and Negative-Ideal Solutions

Solution Type	IDC	QFC	MFC	BPCC	BTEACC
Ideal	0.1662	0.1609	0.1614	0.1662	0.1603
Negative-Ideal	0.0459	0.0473	0.0516	0.0377	0.0520

Table-6: Separation Measures

Alternative	Separation from Ideal	Separation from Negative
CF	0.2425	0.0179
DCE	0.2602	0.0000
DCM	0.2470	0.0164
DMSO	0.0000	0.2602
DMF	0.2008	0.0619

Table-7: Closeness Coefficient and Final Ranking

Alternative	Closeness Coefficient	Rank
DMSO	1.0000	1
DMF	0.2355	2
CF	0.0687	3
DCM	0.0623	4
DCE	0.0000	5

4. Conclusion

The present study employed the TOPSIS method, a robust multi-criteria decision-making technique, to objectively evaluate and rank five different solvents—CF, DCE, DCM, DMSO, and DMF—based on their performance in the oxidation of tryptophan by chromium metal complexes. By incorporating five key parameters (IDC, QFC, MFC, BPCC, and BTEACC), each solvent's suitability was quantitatively assessed. The analysis revealed that DMSO possesses the highest closeness coefficient to the ideal solution, making it the most effective solvent among those studied. DMF followed as the second-best alternative, while DCE ranked lowest, indicating comparatively poor performance. This conclusion provides valuable insight for researchers and chemists in selecting optimal solvents for biochemical oxidation processes involving chromium complexes. The application of the TOPSIS method demonstrates how multi-criteria analysis can enhance decision-making in chemical research, ensuring more rational, data-driven outcomes.

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