Attribute based Coding, Ranking and Selection of Nanomaterial: A MADM Approach

Tanvir Singh, V.P. Agrawal

Abstract—**Optimum selection of a nanomaterial for research and development of nanoproducts for given application satisfying desired aims and objectives is a multiple attribute/criteria/objective decision making problem. Selection of most appropriate nanomaterial is a very important task in design process or manufacturing of every nanoproduct. There is a need for simple, systematic, and logical methods or mathematical tools to guide decision makers in considering a number of selective attributes and their interrelations and in making right decisions. The paper proposes technique for order preference by similarity to ideal solution to evaluate and rank nanomaterial in the presence of multiple attributes for solving the nanomaterial selection problem. The paper presents attribute based characterization of nanomaterial method for computer storage and retrieval as knowledgebase. The knowledgebase permits in-depth understanding and comparison between nanomaterial available with the scientists and product developers to satisfy their research and development needs. The method normalizes attributes of nanomaterial to nullify the effect of different units and their values in the range of 0 to 1. The relative importance of different nanomaterial attributes for different applications is considered. The weight vector is derived using Eigen value formulation. The positive and negative benchmark solutions for nanomaterial are derived. Euclidean distance of alternatives from these best and worst solutions of nanomaterial leads to the development of proximity /goodness/suitability index for ranking of nanomaterial. Final decision is taken by decision makers on the basis of Strength, Weakness, Opportunity, and Threat analysis and short and long term strategies of the organisation. The methodology is illustrated with the help of an example and step-by-step procedure. Results, discussion, and conclusion, highlight the importance of the proposed methodology**

Index Terms—**Nanomaterial selection; Pertinent attributes; MADM; TOPSIS; Ranking;**

I. INTRODUCTION

An ever increasing variety of nanomaterial is available today, with each having its own characteristics, applications, advantages, and limitations. When selecting nanomaterial for engineering designs, a clear understanding of the functional requirements for each individual component is required and various important criteria or attributes need to be considered. Nanomaterials selection attributes is defined as attribute that influences the selection of a nanomaterial for a given application. These attributes include: physical properties, electrical properties, magnetic properties, mechanical properties, chemical properties, manufacturing properties, nanomaterial cost, product shape, nanomaterial impact on environment, availability, fashion, market trends, cultural aspects, aesthetics, recycling, target group, etc. Nanomaterials selection is one of the most challenging issues in the design and development of structural elements and it is also critical for the success and competitiveness of the manufacturing organisation.

The ability to select the most appropriate nanomaterial for a given application is the fundamental challenge faced by the design engineer. Selection of the appropriate nanomaterial is an integral part of successfully implementation of an engineer's design. A systematic and efficient approach to nanomaterial selection is necessary in order to select the best alternatives for a given application [1–5]. The importance of nanomaterial selection in engineering design has been well recognized. The design decision-making regarding selecting appropriate nanomaterial is dictated by the specific requirements of an application, often the requirements on nanomaterial properties [6]. Recent developments in design, selection of nanomaterial play an important role for engineers. The core objective of nanomaterial selection procedure is to identify the nanomaterial selection attributes and obtain the most appropriate combination of nanomaterial selection attributes in conjunction with the feasible requirements [7]. The selection decisions are complex, as nanomaterial selection is more challenging today.

Thus, efforts need to be extended to identify those attributes that influence nanomaterial selection for a given engineering design to eliminate unsuitable alternatives, and to select the most appropriate alternatives using simple and logical methods. Materials science and engineering plays a vital role in this modern age of science and technology. Various kinds of nanomaterial are used in different sectors, such as housing, agriculture and transportation, etc. to meet the society's requirements. The rapid developments in the field of quantum theory of solids atom manipulation, etc. have opened vast opportunities for better understanding and utilization of various nanomaterials. The improper selection of nanomaterial, result in loss of productivity and profitability and hence reputation of a manufacturing organization. The selection of nanomaterial is not restricted to technical aspects only, but focus also made on environmental considerations. The complexity of nanomaterial selection makes multi-criteria analysis an invaluable tool in the engineering

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design process. There has been rapid increase in the number of nanomaterial and nanomaterial manufacturers. Nanomaterials with vastly different capabilities and specifications are available for a wide range of applications. The selection of the nanomaterial to suit a particular application and production environment, from the large number of nanomaterial available in the market today has become a difficult task. Various considerations such as availability, recycling, production method, disposal method, design life need to be considered before a suitable nanomaterial is selected. To meet the challenges, industries have to select appropriate production strategies, product designs, production processes, work and tool materials, machinery and equipment, etc. Since decision-making is a complex process for that there is a need for simple, systematic, and logical methods or mathematical tools to guide decision makers in considering a number of selection attributes and their interrelations. The aim of the present paper is to propose a Multiple Attribute Decision Making approach to deal with the decision making problems of both qualitative and quantitative attributes for the ranking and optimum selection of nanomaterial. A ranked value judgment on a technique for order preference by similarity to ideal solution (TOPSIS) scale or on a graphical scale for the candidate nanomaterial is introduced. The proposed method helps the decision maker to arrive at a decision based on either the ranking of the candidate nanomaterial based on technique for order preference by similarity to ideal solution (TOPSIS) method or based on the graphical methods for easy comparison with importance of constraints for the application to be considered for nanomaterial selection.

In the past lot of research had been reported for selection of material using classical multi attribute decision-making methods. A multi attribute analysis is a popular tool to select best alternative for given applications and the methods are simple additive weighted (SAW) method, weighted product method (WPM), technique for order preference by similarity to ideal solution (TOPSIS), analytical hierarchy process (AHP), graph theory and matrix representation approach (GTMA), etc. Various approaches had been proposed to address the issues of material selection. Rao and Davim [7] proposed TOPSIS method combined with AHP for material selection. Shanian and Savadogo O [8] presented material selection models using a multiple attribute decision making (MADM) method known as ELECTRE. However, ELECTRE method uses the concept of outranking relationship and the procedure is rather lengthy. Only a partial prioritization of alternative materials is computed in ELECTRE models. Shanian A, Savadogo O [9] applied ELECTRE IV for a non-compensatory compromised solution for material selection of bipolar plates for polymer electrolyte membrane fuel cell (PEMFC). Shanian and Savadogo [10] applied TOPSIS method as multiple-criteria decision support analysis for material selection of metallic bipolar plates for polymer electrolyte fuel cell.

However, the TOPSIS method proposed by them does not take into account the qualitative nature of the material selection attributes. Rao et al. [11] presented improved compromise ranking method for material selection known as VIKOR. Wang and Chang [12] emphasized a fuzzy multiple criteria decision-making approach to help selecting the best suited tool steel material for a specific manufacturing application. Liao [13] took the advantage of a fuzzy multi-criteria decision-making method for material selection. Chen and Hwang [14] proposed, GTMA to find out the relative importance between attributes using 8-scales. Hwang CL and Yoon KP [15] illustrate various multiple attribute decision-making: methods and applications. Rao et al. [16, 17] presented a material selection model using graph theory and matrix approach. However, the method does not have a provision for checking the consistency in the judgments of relative importance of the attributes. Manshadi et al. [18] proposed numerical method for the material selection combining non-linear normalization with modified digital logic method. However, the method does not make a provision for considering the qualitative material selection attributes. Chan and Tong [19] proposed weighted average method using grey relational analysis to rank the materials with respect to certain quantitative attributes. Chatterjee et al. [20] used compromise ranking and outranking methods for material selection. The material selection is carried out using fuzzy decision-making, material design and selection using multi objective decision-making methods [21, 22]. Suresh et al. [23] used the TOPSIS method and had considered attributes weight according to an importance and capability of materials.

The literature review indicates the absence of any contribution in the area of nanomaterial selection. During the past few years, fast-changing technologies on the nanoproducts front have created fast response from the industries. Keeping in view of the above research works on material selection, a novel decision making method is proposed in this paper for nanomaterial selection for a given engineering design application. The paper attempts to solve the nanomaterial selection problem using the most potential multi-attribute decision-making (MADM) approach by comparing the relative performance of candidate nanomaterial with the +ve benchmark nanomaterial and select the nanomaterial which is closest to the ideal solution.

The approach is a combination of both technique for order preference by similarity to ideal solution (TOPSIS) and multiple attribute decision making (MADM) which has a high potential to select a best possible alternative from several alternatives according to various criteria. The paper presents a representative nanomaterial database and a transparent assessment procedure, which help the completion of the selection process by focusing on efficiency and consistency.

II. Identification of Nanomaterial attributes

Proper identification of nanomaterial attributes is critically important when comparing various alternative nanomaterials. However, in most cases the user needs to be assisted in identifying the nanomaterial attributes wisely as per the considered application. The final nanoproduct of industry is directly depends on the proper choice of the nanomaterial.

General Attributes	
1. Malleability	2. Polymorphism
3. Ductility	4. Surface topology
5. Durability	6. Molecular weight
7. Stiffness	8. Conductivity of electricity
9. Granularity	10. Dimensional stability
11. Colour	12. Magnetic ordering
13. Resistance to deformation	14. Specific surface area
15. Crystal phase	16. Rigidity
17. Wear resistance	18. Film friction coefficient
19. Current density	20. Toughness
21. Dispersion	22. Metallic behaviour
23. Aspect ratio	24. Stability
25. Solubility	26. Resistance high temperature
27. Robustness	28. Angle of incidence
29. Crystal structure	30. Work function
Physical Attributes	
31.Density	32. True density
33. Specific suspension	34. Melting point
35. Resilience	36. Boling point
37. Bulk density	38. Decomposition temperature
39. Molar heat capacity	40. Lattice constant
41. Catalyst	42. Gas solid liquid
43. Diameter	44. Morphology
45. Particle size	46. Emissivity
47. Purity	48. Hardness
49. Length	50. Short term beam stability
Mechanical Attributes	
51.Tensile strength	52. Compression yield strength
53. Young's modulus	54. Coefficient of friction
55. Shear modulus	56. Flexural strength
57. Bulk modulus	58. Poisson's ratio
59. Impact strength	60. Van der wall forces
61. Internal surface area	62. Fracture toughness
Atomic Attributes	
63.Oxidation states	64.Atomic radius
65.Electro-negativity	66.Covalent radius
67 Ionization energies	68.Van der wall radius
Electrical Attributes	
69. Electrical resistivity	70. Electrical performance
71. Dielectric constant	72. Superconductivity
73. Dielectric strength	74. Conductance quantization
75. Band structure	76. Band gap
77. Curvature effects	78. Electrical conductivity
Thermal Attributes	
79. Thermal conductivity	80. Thermal stability
81. Thermal expansion	82. Specific heat
83. Coefficient of thermal expansion	84. Temperature
85. Ballistic conductance	86. Temperature stability
87. Standard enthalpy of formation	88. Nucleation
Optical Attributes	
89. Transmission	90. Absorption
91. Luminescence	92. Photo-luminescence
93. Index of refraction	94. Surface Plasmon
95. Oscillation	96. Relaxation time

Table-1.list of broad categories of nanomaterial attributes.

. For this purpose, cause and effect analysis diagram is drawn to identify all the different attributes and other parameters of nanomaterial, which require attention/situation of designer's, researchers, industrialists and manufacturers, etc. in the subject area under consideration. The cause and effect diagram for identification of attributes for nanomaterial characterization are shown in **Figure 1.**

The nanomaterial attributes are identified based on its broad area as general parameters, physical parameters, mechanical parameters, atomic parameters, electrical parameters and thermal parameters, etc. are shown in **Table 1**.

The above 96 attributes are useful for storage, retrieval, designing, manufacturing, evaluation, ranking and optimum selection of nanomaterial for research and development **(R & D)** of a nanoproducts. Out of 96 identified attributes, there are '**30**' attributes in general, '**20**' attributes in physical, '**12**' attributes in mechanical, '**6**' attributes in atomic, '**10**' attributes in electrical, '**10**' attributes in thermal, and remaining '**8**' attributes in optical categories.

2.1. Quantification and measurement of the attributes

The nanomaterial are expressed in detailed manner with the attributes identified, e.g. Young's modulus 107 Gpa, Tensile strength >55 Gpa, Aspect ratio 1000, etc. But all these attributes are not quantitative, e.g. band structure, morphology, etc. The nanomaterial is rated on the scale of 0-5 for these attributes.

A similar approach has to be used for the informative attributes, which just tells the information about some attributes of the nanomaterial, such as structure of the nanomaterial or the density of nanomaterial, etc, which is denoted by some number whose numerical value has no significance. It cannot be used for the mathematical treatment, since it is just a numeric representation.

There are some attributes of which quantification is not readily available and has to be done by some mathematical modeling, simulation and analysis. In many cases, the manufacturer make it a standard practice to identify, quantify and provide the information of these attributes which is helpful for nanomaterial designer, manufacturers, industrialists, and users, etc.

A. Usefulness to the manufacturer

The quantification and monitoring of the attribute magnitudes helps the manufacturer to control them closely to fulfil the demand of the user precisely. Moreover, it also helps to find out the market trend by observing the attributes magnitudes. It helps the manufacturer to modify their product to suit the future needs of the nanomaterial users. The data is used to produce optimum nanomaterial in the minimum possible time.

The nanomaterial manufacturer uses these attributes for the **SWOT** (Strength–Weakness–Opportunity–Threat) analysis of nanomaterial products.

B. Usefulness to the designer

For the designer at conceptual design stage, identification of attributes helps to generate various alternative designs, which are developed as modular nanomaterial. Using the modular nanomaterial approach, the optimum nanomaterial according to the market requirements are designed in short time. The critical attributes, which directly affects the

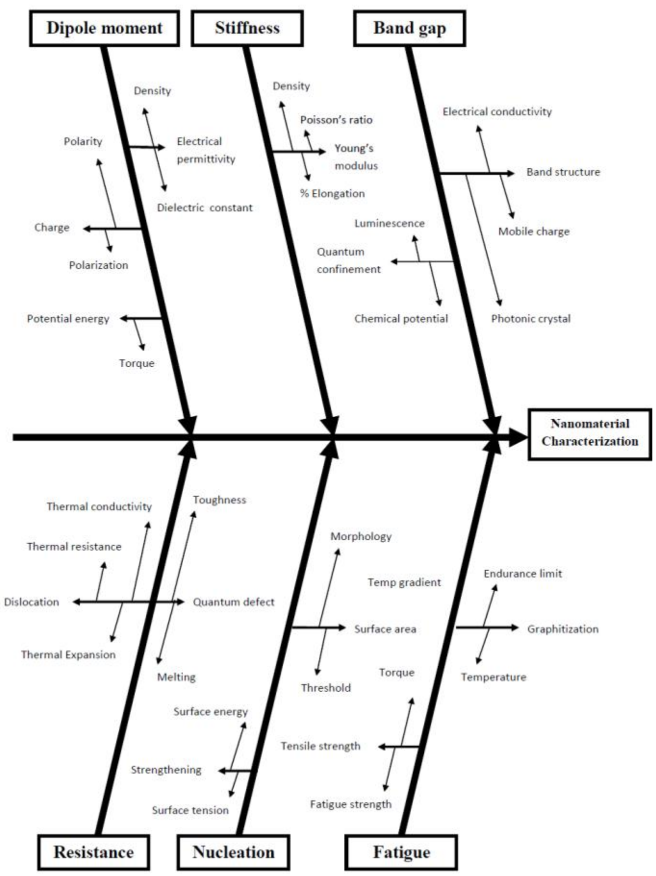

Fig-1.Identification of attributes for nanomaterial characterization

C. Usefulness to the user

Identification of the attributes helps the user for the data storage and their retrieval. The computerized data is generated in different formats for different purposes by different peoples in the organization. It helps the user to select the best possible nanomaterial for the particular application, whenever it is required.

Keeping the short term and long term objectives in mind, comprehensive strength, weakness, opportunity, and threat (SWOT) analysis by the designer, device manufacturer, and research and development (R & D) organizations helps in the development of creative and innovative nanoproducts.

2.2. Coding Scheme of Nanomaterial Attributes

In order to facilitate the selection of pertinent attributes for the application, the attributes are required to be evaluated and coded for range of values. Coding is alphanumeric. The attributes are of two types: quantitative/deterministic and qualitative/fuzzy/subjective. Quantitative attributes determined are calculated using mathematical models or experimentally. Qualitative attributes are subjective in nature and imprecise information is available. It is desirable to evaluate the existence of both types of attributes on one of the several interval scales 0-5 for uniformity. Quantification of many of these attributes is not readily available from the manufacturer. A team of experts from relevant disciplines codifies all the attributes related to a particular nanomaterial based on the application that is to be considered. The illustration of proposed coding scheme for quantitative and qualitative attributes is shown in **Table 2.**

Quantitative Attributes				Qualitative Attributes			
SSA (Kg/m^3)	Code	TS (GPa)	Code	MO	Code	Morphology	Code
25 Kg/m^3	0	10 GPa	0	Not available	0	Cubic	CU
50 Kg/m^3	1	20 GPa	1	Magnetic	M	BCC	B
100 Kg/m^3	2	30 GPa	2	Diamagnetic	D	FCC	F
150 Kg/m^3	3	40 GPa	3	Paramagnetic	P	Cylindrical	CY
200 Kg/m^3	4	50 GPa	4			Tubular	T
>250 Kg/m^3	5	>60GPa	5			Pseudo hexa	P

Note: SSA: Specific Surface Area; TS: Tensile Strength; MO: Magnetic Ordering;

Table-2.coding scheme for quantitative and qualitative attributes of nanomaterial

The table illustrates the coding scheme of qualitative and quantitative attributes. The codes represent the coding of specific surface area of the nanomaterial in the respective shell number **14,** as shown in table 3. Here, the nanomaterial under consideration has the specific surface area of 290 Kg/m^3 which is given a code of **'5'** as shown in table 4.Similarly the coding of morphology of nanomaterial, which is represented by respective shell number **'44'** as shown by table 3. The nanomaterial under consideration has the morphology of tubular structure given a code **'T'** as shown by table 4.

The above mentioned attributes are tabulated in the form of 96-digit coding scheme for characterization of nanomaterial as shown in **Table 3**.

General	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Physical	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
	46	47	48	49	50										
Mechanical	51	52	53	54	55	56	57	58	59	60	61	62			
Atomic	63	64	65	66	67	68									
Electrical	69	70	71	72	73	74	75	76	77	78					
Thermal	79	80	81	82	83	84	85	86	87	88					
Optical	89	90	91	92	93	94	95	96							

Table-3.96-digit coding scheme for characterization of nanomaterial

Example of coding scheme of standard nanomaterial "Q Tubes® 250" are shown in **Table 4.**

Coding scheme for all the 96 attributes is presented for the standard nanomaterial under consideration. All these attributes for **"Q Tubes® 250"** nanomaterial is collected from different research publications and some of them from commercial products and applications, table 4 clearly indicates that the information supplied by the manufacturer to the user is meagre and it is required to be more elaborate.

S/No	Attributes	Information	Code
1	Malleability	-	0
2	Polymorphism	None	N
3	Ductility	-	0
4	Surface topology	-	0
5	Durability	Less	1
6	Molecular weight	-	0
7	Stiffness	-	0
8	Conductivity of electricity	-	0
9	Granularity	-	0
10	Dimensional stability	Stable	4
11	Colour	Black	B
12	Magnetic ordering	Diamagnetic	D
13	Resistance to deformation	-	0
14	Specific surface area	290 Kg/m^3	5
15	Crystal phase	Amorphous Highly Crystalline	A
16	Rigidity	-	0
17	Wear resistance	-	0
18	Film friction coefficient	-	0
19	Current density	>3.2x10^{9}A/cm^2	5
20	Toughness	-	0
21	Dispersion	Soluble in Organic Solvents	3
22	Metallic behaviour	-	0
23	Aspect ratio	~1000	5
24	Stability	Stable	S
25	Solubility	In-soluble	IS
26	Resistance to high temperature	-	0
27	Robustness	-	0
28	Angle of incidence	Amorphous highly Crystalline	5
29	Crystal structure	-	0
30	Work function	-	0
31	Density	-	0
32	True density	~2.1g/cm^3	4
33	Specific suspension	Dispersions in water	W
34	Melting point	3652-3697 °C	5
35	Resilience	-	0
36	Boling point	-	0
37	Bulk density	0.20g/cm^3	5
38	Decomposition temperature	-	0
39	Molar heat capacity	-	0
40	Lattice constant	-	0
41	Catalyst	Slight Impurities < 5% catalyst	3
42	Gas solid liquid	Physical State Solid Amorphous	P
43	Diameter	Average Outer-inner Diametre12nm-8nm,	5
44	Morphology	Tubular Structure	T
45	Particle size	-	0
46	Emissivity	-	0
47	Purity	>95% by weight	4
48	Hardness	-	0
49	Length	4-5 micrometer	4
50	Short term beam stability	-	0
51	Tensile strength	400GPa	5
52	Compression yield strength	-	0
53	Young's modulus	107 GPa	5
54	Coefficient of friction	-	0
55	Shear modulus	-	0
56	Flexural strength	-	0
57	Bulk modulus	-	0
58	Poisson's ratio	-	0
59	Impact strength	-	0
60	Van der wall forces	0.2cm	2
61	Internal surface area	-	0
62	Fracture toughness	-	0
63	Oxidation states	-	0
64	Atomic radius	-	0
65	Electro-negativity	-	0
66	Covalent radius	-	0
67	Ionization energies	-	0
68	Van der wall radius	-	0
69	Electrical resistivity	-	0
70	Electrical performance	Conducting	C
71	Dielectric constant	-	0
72	Superconductivity	-	0
73	Dielectric strength	-	0
74	Conductance quantization	-	0
75	Band structure	-	0
76	Band gap	-	0
77	Curvature effects	-	0
78	Electrical conductivity	>100 Simens/cm (Along Tube Axis)	5
79	Thermal conductivity	>3000 W/m-K (Along Tube Axis)	5
80	Thermal stability	-	0
81	Thermal expansion	-	0
82	Specific heat	-	0
83	Coefficient of thermal expansion	-	0
84	Temperature	-	0
85	Ballistic conductance	-	0
86	Temperature stability	2800 °C in vacuum and 780 °C in Air	4
87	Standard enthalpy of formation	-	0
88	Nucleation	-	0
89	Transmission	-	0
90	Absorption	-	0
91	Luminescence	-	0
92	Photo-luminescence	-	0
93	Index of refraction	-	0
94	Surface Plasmon	-	0
95	Oscillation	-	0
96	Relaxation time	0.8 sec	1

Table-4.coding scheme for standard nanomaterial '**Q tubes® 250'**

Most of the cells are having 0 as code in them. The '0' represents that the information relating to the particular cell is not available to the authors. Information is to be provided by the manufacturer to complete the database. Moreover, the data storage, retrieval and the selection procedure is more precise and accurate.

Tabular representation of coding scheme for standard nanomaterial '**Q Tubes® 250'**is done in compact way as shown in **Table 5**.

General	1	N	3	4	1	6	7	8	9	4	B	D	13	5	A
	16	17	18	5	20	3	22	5	S	IS	26	27	5	29	30
Physical	31	4	W	5	35	36	5	38	39	40	3	P	5	T	45
	46	4	48	4	50										
Mechanical	5	52	5	54	55	56	57	58	59	2	61	62			
Atomic	63	64	65	66	67	68									
Electrical	69	C	71	72	73	74	75	76	77	5					
Thermal	5	80	81	82	83	84	85	4	87	88					
Optical	89	90	91	92	93	94	95	1							

Table-5. Tabular representation of coding scheme for standard nanomaterial '**Q tubes® 250'**

The alphabets used in the coding scheme for standard nanomaterial has unique information in itself. The nanomaterial which is taken into consideration are of black colour is represented by letter 'B', Similarly, all the basic properties of standard nanomaterial are represented as like: the considered standard nanomaterial '**Q Tubes® 250'**is stable in nature is represented by 'S', insoluble in nature is represented by 'IS', polymorphism not done is represented by 'N', magnetic ordering of diamagnetic in nature is represented by 'D' and having a amorphous crystal phase is represented by 'A', physical in nature is represented by 'P', having morphology of tubular structure is represented by 'T'. For this specific suspension/dispersion in water is represented by 'W', having electrical performance conduction is represented by 'C'. Rest of numerical codes are given on the basis of their relative importance, highest code, i.e. '5' to highly important attributes and lesser code like '4', and '3' to less important attributes and '2','and '1' to very less important attributes and '0' for totally absent attributes. The coding scheme is also used for the visual comparison between two nanomaterials up to certain extent. It allows faster comparison in various formats.

III. Stage Optimum Selection Procedure

The procedure permits faster convergence to optimum selection of nanomaterial for given application which is to be considered.

Stage-1 Elimination Search Method

All the attributes are not equally important, while selecting the nanomaterial for particular application. There are few attributes, which have direct effect on the selection procedure. Pertinent attributes as necessitated by the particular application and/or the user are identified. The threshold values to these 'pertinent attributes' are assigned by obtaining information from the user and the group of experts. Henceforth, the selection procedure focuses solely on the pertinent attributes leaving out the rest. On the basis of the threshold values of the pertinent attributes, a shortlist of nanomaterial is obtained, which satisfies minimum, maximum, and target values of the pertinent attributes. To facilitate that search procedure an identification system has been made for all the nanomaterial in the data.

Stage-2 Evaluation Using TOPSIS Method

Step-1 Decision matrix

The first step is to represent all the information available from the data about these satisfying solutions in the matrix form. Such a matrix is called decision matrix 'D' [d_{ij}]. Each row of the matrix is allocated to one candidate nanomaterial and each column to one attribute under consideration. An element 'd_{ij}' of the decision matrix D gives the value of j^{th} attribute in the row (non-normalized) form and units for the i^{th} nanomaterial. Thus if the number of short-listed nanomaterial is 'm' and the number of pertinent attributes is 'n' the decision matrix is an 'm x n' matrix.

Step-2 Normalized specifications matrix

The second step is construction of the normalized specification matrix, 'N' [N_{ij}] from the decision matrix D. Normalization is used to bring the data within particular range 0 to 1 and moreover, it provides the dimensionless magnitudes. The phenomenon is used to calculate the normalized specification matrix. The normalized specification matrix has the magnitudes of all the attributes of the nanomaterial on the common scale of 0 to 1. It is a sort of value, which indicates the standing of that particular attribute magnitude when compared to the whole range of the magnitudes for all candidate nanomaterial.

An element n_{ij} of the normalized matrix N be calculated as:-

$$n_{ij} = d_{ij} \Big/ \left(\sum_{i=1}^{m} d_{ij}^2 \right)^{1/2} \qquad \text{Where } d_{ij} \text{ is an element of the decision matrix, D} \qquad (1)$$

Step-3 Relative Importance Matrix

The third step is to obtain information from the user or the group of experts of area related to nanomaterial to calculate the relative importance of one attribute with respect to another. The information is sought in terms of a ratio. Information on all such pair-wise comparisons is stored in a matrix called as relative importance matrix 'A' [a_{ij}], which is 'n x n' matrix. Here 'a_{ij}' contain the relative importance of i^{th} attribute over the j^{th} attribute. The symmetric terms of the matrix are reciprocals of each other, while the diagonal elements are unity. The information stored in matrix 'A' is on pair-wise basis. It is modified into representation that gives the relative weights of all attributes taken together, so that the cumulative sum of the weights is equal to unity.

Step-4 Find out the maximum Eigen value of the relative importance matrix A.

The Eigen vector method, which modifies inconsistencies in the judgement of relative importance of attributes while making pair-wise comparisons, is used to find out the weights. These inconsistencies arise due to inaccurate human judgments [24]. The Eigen vector method seeks to find weight vector 'W' from the Eigen value problem associated with the matrix 'A'. If,

$$W = \begin{bmatrix} W1 \\ W2 \\ . \\ . \\ . \\ W5 \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} a11 & a12 & ...... & a1n \\ a21 & a22 & ...... & a2n \\ ...... & ..... & ...... & ..... \\ ...... & .... & ..... & .... \\ ..... & ..... & ..... & ..... \\ an1 & an2 & ...... & ann \end{bmatrix} \qquad (2)$$

Then the linear transformation Y = AW

Transforms the column vector 'W' into the column vector 'Y' by means of the square matrix 'A'. In practice, it is often required to find such vectors which transform them into themselves or to a scalar multiple of themselves.

Let W be such a vector which transforms into λW by means of the transformation equation. Then, $A W = \lambda W$ or

$$AW - \lambda IW = 0 \text{ or } (A - \lambda I)\, W = 0 \qquad (3)$$

Where 'λ' the Eigen value of 'A', 'I' is the identity matrix and 'W' is the corresponding Eigen vector [25]. For 'n x n square matrix A' there are 'n' Eigen values λ_i, for i = 1,. . .,n, and corresponding to λ_i, there are 'n' Eigen values. Vector 'W' is now found in the following manner. The Equation (3) is also called Eigen value

The Equation (3) is also written as $(A - \lambda\, I) = 0$ (4)

& W = 0, where W = 0, gives a trivial solution having no meaning.

Take Eigen weight vector, W corresponding to the largest Eigen value λ_{max}, as all the elements of λ are either positive or negative. [24]. In this way, maximum Eigen value is calculated by using Equation (4).

Step-5.Calculating weights for each attribute using the Eigen vector associated with maximum Eigen value.

In order to find out the weights for each attribute using Eigen vector associated with maximum Eigen value is calculated by using Equation (5) as:-

$$(A - \lambda_{max}\, I)\, W = 0 \qquad (5)$$

In this summation of weight vectors W_i is given as:-

$$\sum_{i=1}^{n} w_i = 1. \qquad (6)$$

$$w_1 + w_2 + w_3 + w_4 + w_5 = 1 \qquad (7)$$

Step-6 Weighted normalized specification matrix

The weights obtained from the relative importance matrix have to be applied to the normalized specifications since all attributes have different importance while selecting the nanomaterial for particular application. The matrix, which combines the relative weights and normalized specification of the candidates, is weighted normalized matrix, 'V'. It gives the true comparable values of the attributes is obtained as follows:-

$v_{ij} = w_j \cdot n_{ij}$, i = 1,……,m and j = 1,…….,n

$$\mathbf{V} = \begin{bmatrix} w_1 n_{1,1} & w_2 n_{1,2} & \cdots & w_n n_{1,n} \\ w_1 n_{2,1} & \ddots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ w_1 n_{m,1} & w_2 n_{m,2} & \cdots & w_n n_{m,n} \end{bmatrix} = \begin{bmatrix} v_{1,1} & v_{1,2} & \cdots & v_{1,n} \\ v_{2,1} & \ddots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ v_{m,1} & v_{m,2} & \cdots & v_{m,n} \end{bmatrix} \qquad (8)$$

The positive-ideal (best) solution of nanomaterial is expressed as:-

$$V^{+} = \{(\max_i \sum V_{ii} / j \in J), (\min_i \sum V_{ii} / j \in J') / \; i=1,2,3,\ldots\ldots,N\}, \qquad (9)$$
$$= \{V_1^{+}, V_2^{+}, V_3^{+}, V_4^{+}, \ldots\ldots V_M^{+}\}$$

The Negative-ideal (worst) solution of nanomaterial is expressed as:-

$$V^{-} = \{(\min_i \sum V_{ii} / j \in J), (\max_i \sum V_{ii} / j \in J') / \; i=1,2,3,\ldots\ldots,N\}, \qquad (10)$$
$$= \{V_1^{-}, V_2^{-}, V_3^{-}, V_4^{-}, \ldots\ldots V_M^{-}\}$$

Where J = (j=1,2,3……,M) / j is associated with beneficial attributes, and J'=(j=1,2,3……,M) / j is associated with non-beneficial attributes. The alternative V^+ indicates the most preferable alternative or the ideal solution. Similarly, alternative V^- indicates the least preferable alternative or the negative-ideal solution.

Step-7.Generation of +ve and –ve benchmark nanomaterial and separation measures

The weighted normalized matrix V is used to obtain the +ve and –ve benchmark nanomaterial, where the both benchmark nanomaterial are hypothetical nanomaterial, which supposed to have best and worst possible attribute magnitudes. The TOPSIS method is based on the concept that the chosen option (optimum) have the shortest distance from the +ve benchmark nanomaterial (best possible nanomaterial) and be farthest from the –ve benchmark nanomaterial (worst possible nanomaterial). The measure ensures that the top ranked nanomaterial is closest to +ve benchmark nanomaterial and farthest from –ve benchmark nanomaterial. The calculations are made on separation measures from +ve and –ve benchmark nanomaterial, respectively, as S^+_i and S^-_i.

The separation of candidates from the +ve benchmark nanomaterial is given by:-

$$S_i^{+} = \left\{ \sum_{j=1}^{n} (V_{ij} - V_j^{+})^2 \right\}^{0.5}; \qquad (11)$$
$$j = 1, 2, \ldots, n; \quad i = 1, 2, \ldots, m$$

Separation of candidates from the -ve benchmark nanomaterial is given by:-

$$S_i^{-} = \left\{ \sum_{j=1}^{n} (V_{ij} - V_j^{-})^2 \right\}^{0.5}; \qquad (12)$$
$$j = 1, 2, \ldots, n; \quad i = 1, 2, \ldots, m$$

Step-8.Suitability Index

Then the relative closeness of candidates to the +ve benchmark nanomaterial, C_i*, which is a measure of the suitability of the nanomaterial for the chosen application on the basis of attributes considered, is calculated. A nanomaterial with the largest C_i* is preferable

$$C_i^* = \frac{S_i^-}{S_i^+ + S_i^-} \quad \text{Where } i = 1, \ldots\ldots\ldots\ldots, m \qquad (13)$$

Ranking of the candidate nanomaterial is done in accordance with the decreasing values of indices C_i*, indicating the most preferred and the least preferred feasible optional solutions, this index is called suitability/goodness/proximity index.

The multiple attribute decision making (MADM) methods choose or rank finite number of alternatives that are measured by a few relevant attributes. The technique for order preference by similarity to ideal solution (TOPSIS) is the technique used to rank these alternatives in the presence of multiple attributes representing a candidate nanomaterial. The technique is illustrated with the help of an example in the later section.

3.1. Graphical method based ranking

There are many methods to evaluate the nanomaterial using mathematical approach [24]. A graphical method is proposed to process the available data and select the nanomaterial. The graphical representation methods, like line graph are used for this purpose.

3.1.1. Line graph representation

The specification matrix D, normalized and weighted normalized specification matrices N and V, respectively, containing information of the candidate nanomaterial are developed. These matrices are represented graphically using line graph by plotting the magnitude of the attributes on the vertical axis and the attributes on the horizontal axis. The values are plotted for different candidate nanomaterial to obtain the line graph for them. These graphs are distinct for all of the candidate nanomaterial and used for comparison. The area under the curve used for quantification purpose and to compare the candidate nanomaterial with each other.

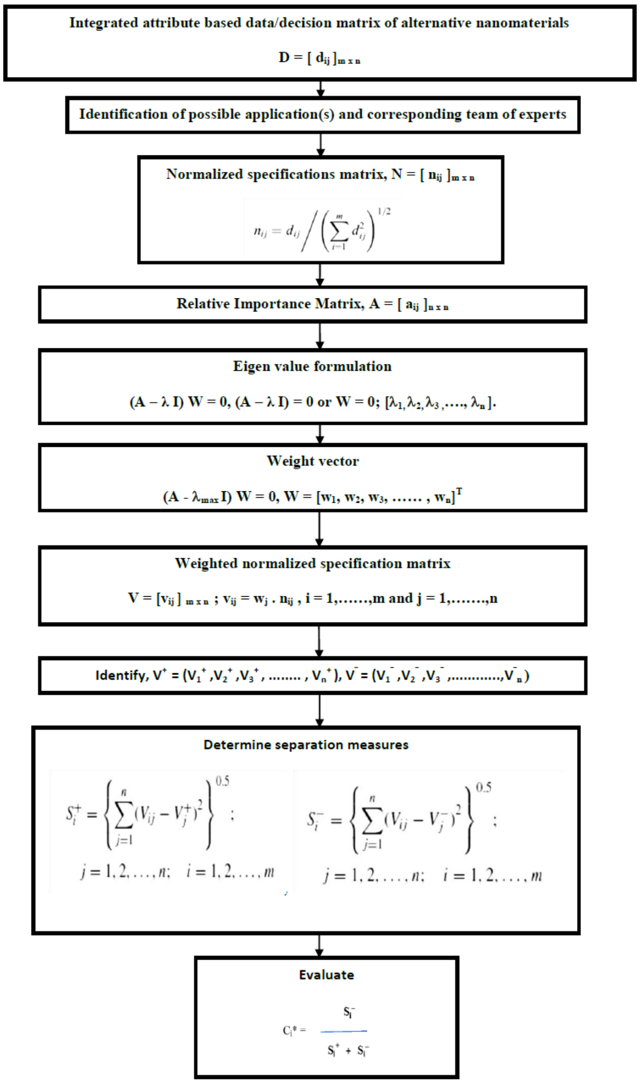

Fig-2.TOPSIS flow chart

The line graphs are plotted for specifications, normalized and weighted normalized specifications of all the candidate nanomaterial as well as the benchmark nanomaterial. The area under the curve is obtained as follows.

Let the width between the two parameters on horizontal axis as unity and d_{ij}, n_{ij}, and v_{ij} are the elements of D, N, and V matrices

Area under the line graph of specification of i^{th} nanomaterial found out as:-

$$AD_i^L = (d_{i,1} + 2(d_{i,2} + \cdots + d_{i,n-1}) + d_{i,n})/2 \qquad (14)$$

Similarly, area under the line graph of normalized and weighted normalized specifications of the i^{th} nanomaterial, i.e. AN_i^L and AV_i^L using their respective elements are obtained.

3.1.1. Identification and graphical representation of the benchmark nanomaterial.

The same +ve benchmark nanomaterial, defined earlier, is used here for the comparison of the candidate nanomaterial for the ranking purpose. The areas under the line graph for +ve benchmark nanomaterial, i.e., AD^L_B, AN^L_B, and AV^L_B, are calculated. All the candidate nanomaterial are compared with the +ve benchmark nanomaterial for the evaluation purpose. It shows the suitability of the nanomaterial for the particular task/applications.

3.1.2. Ranking and selection of the nanomaterial.

Now, specification matrix is used along with normalized specification and weighted specification matrices of all the candidate nanomaterial along with the +ve benchmark nanomaterial. There is a need to measure and compare the candidate nanomaterial with benchmark nanomaterial for ranking and optimum selection.

3.1.3. Coefficient of similarity (COS).

The evaluation and ranking of the nanomaterial using the novel graphical methods is done by their similarity to +ve benchmark nanomaterial. Let the Coefficient of similarity (COS) be the ratio of area under the curve or enclosed by the polygon for the candidate to that of the benchmark nanomaterial. The value of COS be any +ve fraction ($0 \leq COS \leq 1$) and a measure of the closeness of candidate nanomaterial with the benchmark nanomaterial. The candidates with COS magnitude closer to unity are preferable, since it indicates the closeness to the +ve benchmark nanomaterial.

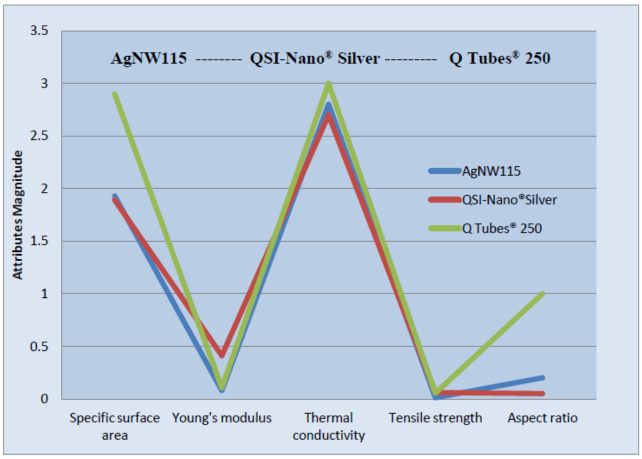

Fig-3 Line graph plot for evaluation and ranking of nanomaterial.

According to TOPSIS method

$COS = (C_i^* - 0)$, $COS^D = (1 - C_i^*)$, and $COS + COS^D = (C_i^* - 0) + (1 - C_i^*) = 1$.

Coefficient of similarity (COS) based on decision matrix

$$COS_j^D = AD_j / AD_I \qquad \textbf{(15)}$$

AD_j and AD_I area under the line graph of specifications for j^{th} and i^{th} nanomaterial

.

Property	Description	Target Value
Specific surface area	Used to determine the type and properties of nanomaterials having large specific surface areas relative to their volumes are more important as per the considered application.	Max = 315kg/m^3
Young's modulus	Measure of the stiffness of nanomaterials and is a quantity used to characterize nanomaterials. Target is highest combination of young's modulus and poisson's ratio.	Min = 58 GPa
Thermal conductivity	Property of a material's ability to conduct heat, an important property for many applications, such as optical nanodetectors and solar thermal stability. High thermal conductivity is important in material science, research, electronics target is highest combination of thermal conductivity and heat transfer coefficient.	Min = 1523W/m-K
Tensile strength	Maximum stress that a material can withstand while being stretched or pulled before necking. Tensile strengths are rarely used in the design of ductile nanomembers, but they are important in brittle nanomembers.	Min = 10 GPa
Aspect ratio	Properties and large aspect ratio of nanomaterials a promising template for bottom-up fabrication of nanodevices and various nanoproducts.	Max = 1000

Table-6. Target nanomaterial properties for manufacturing of nanodevices

Coefficient of similarity (COS) based on normalized specifications matrix

$$COS_j^N = AN_j/AN_I \quad (16)$$

AN_j and AN_I area under the line graph of normalized specifications for ^{jth} and ith nanomaterial.

Coefficient of similarity (COS) based on weighted normalized matrix

$$COS_j^V = AV_j/AV_I \quad (17)$$

AV_j and AV_I area under the line graph of weighted normalized specifications for jth and ith nanomaterial.

Thus the COS calculations for all the 'n' number of candidate nanomaterial are done by graphical methods, viz., line graph methods using the weighted normalized specifications.

IV. ILLUSTRATIVE EXAMPLE OF RANKING AND OPTIMUM SELECTION OF NANOMATERIAL

Scientists, engineers and product developers use the following example for implementation of proposed methodology.

Stage-1.Elimination Search Method

In this stage, firstly identify the application and corresponding pertinent attributes. After identifying the application, define the requirements of research and product development carefully. Then, eliminate the large list of nanomaterial to a manageable list. In order to illustrate the proposed methodology an example is considered for ranking and optimum selection of nanomaterial for **"manufacturing of industrial nanodevice"** taken as an application. As the nanomaterial selection for the manufacturing of nanodevices is based on the various aspects of designing and

Characteristics of the nature of the nanodevices. Nanodevices exhibit a wide variety of electronic behaviours, which includes classical behaviour such as ohmic resistance at low voltage and rectification and less common behaviours, such as negative differential resistance, and hysteretic switching.

The following characteristics/target properties are required for nanomaterial to manufacture nanodevices as follows:-

a) High specific surface area to determine the type and properties of a nanomaterial
b) Young's modulus for measure of the stiffness of nanomaterial and quantity with target highest in combination of young's modulus and poissons ratio,
c) Thermal conductivity property of a material's ability to conduct heat and target is highest combination of thermal conductivity and heat transfer coefficient
d) Tensile strength,
e) Aspect ratio as a promising template for bottom-up fabrication of nanodevices.

In general, in case of nanodevices, motion nanodevices contains the plate, spherical, torroidal, conical, cylindrical, and asymmetrical geometry with maximum specific surface area (Max = 315kg/m^3) because of high surface area of nanomaterial, it helps in heterogeneous analysis and optimization due to which there is guarantee the superior performance capabilities. The efficiency, reliability, power and torque densities, robustness, durability, compactness, simplicity, controllability and accuracy must be maximized while minimizing cost, maintenance, size, weight, volume, and losses. In case of nanodevices, molecular state variables are well correlated with non-volatile memory requirements such as high density, minimum young's modulus, (Min = 58 GPa) and activation energy, which makes them suitable for memory device applications. It is a persistent need of miniaturization of machines with maximum aspect ratio (Max = 1000) of the nanodevices and for energy conversion devices for various engineering applications. In the case, nanomaterial design of nanoscale devices to maximize phonon transport efficiency is the key, including new nanomaterial with high thermal conductivity such as new carbon-based nanomaterial.

The reality, however, is based on limits set by nanomaterial (such as minimum thermal conductivity (Min = 1523W/m-K), mobility, dielectric constant, minimum tensile strength (Min = 10 GPa)), devices (such as gain, fan-out, and parasitic effects), and manufacturing processes (such as yield, critical dimensions, and line width roughness). In order to study and develop them, it is crucial to fully understand the nanomaterial properties and to work for environment and be able to create appropriate models that account for them.

By keeping all this mind, in the elimination search method, the maximum and minimum value of the attributes have been taken according to their range of values that are required as per the considered application and on the basis of this, target value is decided. Only those criteria are selected that satisfy the target values. After this, out of 100 alternatives of the nanomaterial only 5-6 alternatives are selected at the end of this stage which satisfies the max, min, and target. In this aspect ratio (Max = 1000) and specific surface area (Max = 315kg/m^3) is having maximum value, so it is taken as target criterion.

Based upon this the target nanomaterial properties that are required for manufacturing of nanodevices are summarized in **Table-6**.

After defining the target nanomaterial properties, applied the pertinent attributes, and eliminate infeasible nanomaterial (elimination done on the basis of pertinent attributes one by one based on the target value of pertinent attributes) from the available 'n' attributes database/knowledge base and prepare a manageable list of nanomaterial. In this example, 31 standard nanomaterial with 96 attributes related to 31 nanomaterial have been taken for optimum selection of nanomaterial as per the given application.

List of 31 standard nanomaterial available on different websites are shown in **Table-7**

S/No	List of Standard Nanomaterials	References
1	QSI-Nano® Manganese	www.qsinano.com
2	QSI-Nano® Manganese Dioxide Powder	www.qsinano.com
3	QSI-Nano® Nickel	www.qsinano.com
4	AZ Purifiers™	www.enginecontrolsystems.com
5	QSI-Nano® Nickel Oxide Powder	www.qsinano.com
6	QSI-Nano® Silver Powder	www.qsinano.com
7	AgNW-60	www.seashelltech.com
8	QSI-Nano® Silver	www.qsinano.com
9	ThermoSafe Insulated Shipper-VIP	www.nanopore.com
10	BioPure™ Gold Nanoparticles (AUPB)	www.nanocomposix.com
11	QSI-Nano® Copper	www.qsinano.com
12	NanoPore™ HP	www.nanopore.com
13	AgNW115	www.seashelltech.com
14	NanoXact™ AU Nanoparticles	www.nanocomposix.com
15	QGraphene® - 50	www.quantum-materials.in
16	AgNW-115-E	www.seashelltech.com
17	DMSX-II Add-on Silencer	enginecontrolsystems.com
18	Citrate NanoXact™ Gold	www.nanocomposix.com
19	Tannic NanoXact™ Gold	www.nanocomposix.com
20	MERV-15 Cartridge	Clark Filter Clarcor Company
21	Purimufflers™	www.enginecontrolsystems.com
22	QSI-Nano® Copper Powder	www.qsinano.com
23	QSI-Nano® Copper Oxide Powder	www.qsinano.com
24	NanoPore™ HT	www.nanopore.com
25	QSI-Nano® Iron	www.QSINANO.com
26	Tannic BioPure™ Gold	www.nanocomposix.com
27	QSI-Nano® Iron Oxide Powder	www.QSINANO.com
28	QSI-Nano® Silver	www.qsinano.com
29	AgNW60	www.seashelltech.com
30	NanoPore™ HP-150	www.nanopore.com
31	Q Tubes® 250	www.quantum-materials.in

Table-7.List of 31 standard nanomaterials available on different websites

Out of these 31 standard nanomaterials, only 7 nanomaterials with their pertinent attributes are best suited for the given application for the selection of best/optimum nanomaterial and remaining 24 standard nanomaterials are eliminated due to the insufficient significance of their attributes as per the given application. A manageable list of 7 standard nanomaterial with 5 pertinent attributes is formed which best suits as per the given application. The attributes for short listed candidate nanomaterial are shown in table 8**.**

Stage-2.Evaluation using TOPSIS method

Step-1.Formation of decision matrix, 'D'

By using table 8**,** prepare a decision matrix. The matrix contains all the magnitudes of specifications. Rows represent the candidate nanomaterial and the columns represent the pertinent attributes.

In this example, 7 candidate nanomaterial and 5 attributes are considered for given application with their values is listed in Equation (18) as:-

$$D = \begin{bmatrix} 193 & 79 & 2850 & 12 & 205 \\ 212 & 910 & 1870 & 15 & 71 \\ 160 & 1020 & 2520 & 26 & 1000 \\ 189 & 411 & 2730 & 62 & 58 \\ 280 & 60 & 2509 & 50 & 70 \\ 256 & 168 & 1705 & 34 & 150 \\ 290 & 107 & 3000 & 55 & 1000 \end{bmatrix} \quad (18)$$

Attributes for the short listed candidate nanomaterial as per the given application are listed in **Table 8.**

Step-2.Calculating the normalized specification matrix using Equation-(1)

The normalization helps to provide the dimensionless elements of the matrix.

$$N = \begin{bmatrix} 0.3166 & 0.0546 & 0.4314 & 0.1115 & 0.1422 \\ 0.3477 & 0.621 & 0.2831 & 0.1394 & 0.0492 \\ 0.2624 & 0.706 & 0.3815 & 0.2417 & 0.6937 \\ 0.31 & 0.2845 & 0.4133 & 0.5764 & 0.0402 \\ 0.4593 & 0.0415 & 0.3798 & 0.4648 & 0.0485 \\ 0.411 & 0.1162 & 0.2581 & 0.316 & 0.104 \\ 0.4757 & 0.074 & 0.4542 & 0.5113 & 0.6937 \end{bmatrix} \quad (19)$$

Alternate Nanomaterials	SSA kg/m^3	YM GPa	TC W/m-K	TS GPa	AR
AgNW115	193	79	2850	12	205
NanoXact™ AU Nanoparticles	212	910	1870	15	71
QGraphene® - 50	160	1020	2520	26	1000
QSI-Nano® Silver	189	411	2730	62	58
AgNW60	280	60	2509	50	70
NanoPore™ HP-150	256	168	1705	34	150
Q Tubes® 250	290	107	3000	55	1000

Note: SSA: Specific Surface Area; YM: Young's Modulus; TC: Thermal Conductivity; TS: Tensile Strength; AR: Aspect Ratio

Table-8. Attributes for short listed candidate nanomaterials (refer to table-7).

Step-3.Construction of relative importance matrix A

To find out the weight vector for different attributes of nanomaterial for given application, the relative importance matrix is developed. A questionnaire form is prepared explaining the requirements of the application, different scientists, product developers and experts are asked to fill up these forms independently and then average is taken to find out the values of all the off-diagonal elements. The values in the lower diagonal matrix cells are reciprocal of the corresponding values in the cells of upper diagonal matrix. In this respect, process was completed by team of experts/stakeholders. Only pair-wise comparison is permitted in this method. i.e. $a_{ij} = w_i/w_j$, where this ratio represents the relative importance of i^{th} attribute with respect to the j^{th} attribute corresponding to the given application. Relative importance matrix for given application is shown below:-

$$A = \begin{bmatrix} 1 & 1 & 2 & 0.5 & 0.33 \\ 1 & 1 & 0.5 & 2 & 2 \\ 0.5 & 2 & 1 & 3 & 2 \\ 2 & 0.5 & 0.33 & 1 & 0.33 \\ 3 & 0.5 & 0.5 & 3 & 1 \end{bmatrix} \quad (20)$$

Step-4.Find out the maximum Eigen value of the relative importance matrix A

Maximum Eigen value of the relative importance matrix 'A' is calculated by using Eigen value formulation, which provides how to find out the weight vector as shown $(A - \lambda I)$ $W = 0$, Where, I is the identity matrix, and W is the weight vector. The equation is also written as $(A - \lambda I) = 0$ and $W = 0$, but $W = 0$ gives a trivial solution having no meaning.

$$(A - \lambda I) = \begin{bmatrix} 1-\lambda & 1 & 2 & 0.5 & 0.33 \\ 1 & 1-\lambda & 0.5 & 2 & 2 \\ 0.5 & 2 & 1-\lambda & 3 & 2 \\ 2 & 0.5 & 0.33 & 1-\lambda & 0.33 \\ 3 & 0.5 & 0.5 & 3 & 1-\lambda \end{bmatrix} = 0 \quad (21)$$

Characteristics Polynomial Equation

$$-\lambda^5 + 5\lambda^4 - 0.03\lambda^3 + 25.85\lambda^2 + 21.88\lambda + 9.767 = 0$$

After solving the characteristics polynomial equation,

by using the MATLAB λ_{max} is calculated. By solving, 5 values of λ are obtained as shown below:-

$\lambda = 6, -0.2095 \pm 2.2910i, -0.2762 \pm 0.4806i$

From this, $\lambda = 6$ is the maximum value, as by taking the largest λ value the correct equation is obtained. Therefore, $\lambda_{max} = 6$. Now put this value in Equation (21)

$$(A - \lambda_{max} I) = \begin{bmatrix} -5 & 1 & 2 & 0.5 & 0.33 \\ 1 & -5 & 0.5 & 2 & 2 \\ 0.5 & 2 & -5 & 3 & 2 \\ 2 & 0.5 & 0.33 & -5 & 0.33 \\ 3 & 0.5 & 0.5 & 3 & -5 \end{bmatrix} \quad (22)$$

Step-5.Calculating weights for each attribute using the Eigen vector associated with maximum Eigen value

The weights for each attribute are calculated by using the Eigen vector associated with maximum Eigen value as:-

$$(A - \lambda_{max} I)\, W = 0 \quad (23)$$

The Equation (23) gives a set of linear simultaneous equations to calculate weight vector.

$$(A - \lambda_{max} I)\, W = \begin{bmatrix} -5 & 1 & 2 & 0.5 & 0.33 \\ 1 & -5 & 0.5 & 2 & 2 \\ 0.5 & 2 & -5 & 3 & 2 \\ 2 & 0.5 & 0.33 & -5 & 0.33 \\ 3 & 0.5 & 0.5 & 3 & -5 \end{bmatrix} \begin{bmatrix} W1 \\ W2 \\ W3 \\ W4 \\ W5 \end{bmatrix} = 0 \quad (24)$$

The solution of Equation (24) is subject to the constraint,

$$\sum_{i=1}^{n} w_i = 1.$$

The solution provides, $W_1 = 0.1761$, $W_2 = 0.2042$. $W_3 = 0.2668$, $W_4 = 0.2430$, $W_5 = 0.2286$

Step-6.Calculating the weighted normalized specification matrix using Equation (8)

Incorporate the relative importance of the attributes with their normalized value to create unique parameters for the candidate nanomaterial.

$v_{ij} = w_j \cdot n_{ij}$, $i = 1,\ldots\ldots,m$ and $j = 1,\ldots\ldots.,n$

$$V = \begin{bmatrix} 0.0557 & 0.0111 & 0.115 & 0.027 & 0.0325 \\ 0.0612 & 0.1268 & 0.0755 & 0.0338 & 0.0112 \\ 0.0462 & 0.1441 & 0.1017 & 0.0587 & 0.1585 \\ 0.0545 & 0.058 & 0.1102 & 0.14 & 0.0091 \\ 0.0808 & 0.0084 & 0.1013 & 0.1129 & 0.011 \\ 0.0723 & 0.0237 & 0.0688 & 0.0767 & 0.0237 \\ 0.0837 & 0.0151 & 0.1211 & 0.1242 & 0.1585 \end{bmatrix} \quad (25)$$

The weighted normalized specification matrix is all-inclusive matrix, which takes care of the attribute values and their relative importance. So the matrix is able to provide good basis for comparison with each other and with the benchmark nanomaterial.

Step-7.Generation of +ve and –ve benchmark nanomaterial and separation measures

The weighted normalized attributes for the +ve and –ve benchmark nanomaterial are obtained considering, design, manufacturing, cost, safety attributes as:-

The weighted normalized attributes for the +ve benchmark nanomaterial is calculated by taking the largest value from all the columns with respect to all the pertinent attributes in correspondence to their candidate nanomaterial.

Theoretically, best solution of nanomaterial is calculated by using Equation (9),

$$V^{+} = (0.0837, 0.1441, 0.1211, 0.1400, \text{ and } 0.1585) \quad (26)$$

Similarly, the weighted normalized attributes for the –ve benchmark nanomaterial is calculated by taking the smallest value from all the columns with respect to all the pertinent attributes in correspondence to their candidate nanomaterial.

Theoretically, worst solution of nanomaterials is calculated by using Equation (10),

$$v^{-} = (0.0462, 0.0084, 0.0688, 0.0270, \text{ and } 0.0091) \quad (27)$$

Values of Separation from the +ve benchmark nanomaterials, $\mathbf{S_i^{+}}$ and Values of Separation from the -ve benchmark nanomaterials, $\mathbf{S_i^{-}}$ are calculated by using Equation (11) and Equation (12) given below in **Table 9.**

$S^{+}_{1} = 0.2171$	$S^{-}_{1} = 0.0527$
$S^{+}_{2} = 0.1893$	$S^{-}_{2} = 0.1197$
$S^{+}_{3} = 0.0916$	$S^{-}_{3} = 0.2069$
$S^{+}_{4} = 0.1752$	$S^{-}_{4} = 0.1304$
$S^{+}_{5} = 0.2032$	$S^{-}_{5} = 0.0981$
$S^{+}_{6} = 0.1988$	$S^{-}_{6} = 0.0510$
$S^{+}_{7} = 0.1299$	$S^{-}_{7} = 0.1896$

Table-9.values of separation from +ve benchmark nanomaterials to –ve benchmark nanomaterials

Step-8.Suitability Index

The relative closeness to the +ve benchmark nanomaterial C_i* ,which is a measure of the suitability of the nanomaterial for the given application on the basis of attributes considered, is calculated by using Equation (13). A nanomaterial with the largest C_i* is preferable.

Therefore, Relative closeness to ideal solution are:-

$$\begin{aligned} C^*_1 &= 0.1953 \\ C^*_2 &= 0.3873 \\ C^*_3 &= 0.6931 \\ C^*_4 &= 0.4267 \\ C^*_5 &= 0.3255 \\ C^*_6 &= 0.2041 \\ C^*_7 &= 0.5934 \end{aligned} \quad (28)$$

Ranking of the candidate nanomaterial is done in accordance with the decreasing values of indices C_i* indicating the most preferred and the least preferred feasible optional solutions. The index is called suitability/goodness/proximity index. The ranking is done as $C_3^* > C_7^* > C_4^* > C_2^* > C_5^* > C_6^*$ C_1*. All the seven candidate nanomaterial is feasible solutions satisfying minimum, maximum, and target values. Final selection needs other considerations.

Computer Program MATLAB

A matrix laboratory **(MATLAB)** program is developed for performing calculations of above procedure from steps 1-8. The **MATLAB** program developed requires decision matrix 'D' and relative importance matrix 'A' as input and after performing the remaining calculations gives ranking in the form of C^*_i as output.

The selection procedure described in section 4 is iterated for each candidate nanomaterial to arrive at optimum nanomaterial for application under consideration.

Graphical method based Ranking

The element values of weighted normalized specification matrix are used for the line graph plotting. Subsequently, COS is calculated from graphs. The calculated COS is tabulated as follows:-

Suppose, the area under the line graph for weighted normalized specifications of first candidate nanomaterial and for benchmark nanomaterial are $AV_1^{L} = 0.1972$; $AV_{+B}^{L} = 0.5263$. The coefficient of similarity based on the weighted normalized specification of the first candidate nanomaterial is:-

$$COS_1^{VL} = AV_1^{L} / AV_{+B}^{L} = 0.3746 \quad (29)$$

Similarly, closeness of the candidate nanomaterial with the +ve benchmark nanomaterial obtained from TOPSIS and the graphical methods are tabulated as shown in table 10**.** Thus the nanomaterial is ranked in order of preference based on the attributes selected. For the purchase of new nanomaterial, the management use the above ranking effectively to select the nanomaterial, which are best suitable for the application and is based on this set together with other considerations.

Evaluation and ranking of the candidate nanomaterial using TOPSIS and graphical methods are shown in **Table 10.**

Candidate Nanomaterials	TOPSIS- Closeness to the +ve benchmark nanomaterial C_i*	Ranking order based on C_i*	COS based on Line Graph COS^{VL}	Ranking order Based on COS^{VL}
AgNW115 (N_1)	0.1953	7	0.3746	7
NanoXact™ AU Nanoparticle (N_2)	0.3873	4	0.5101	5
QGraphene® - 50 (N_3)	0.6931	1	0.7248	2
QSI-Nano® Silver (N_4)	0.4267	3	0.6513	3
AgNW60 (N_5)	0.3255	5	0.5173	4
NanoPore™ HP-150 (N_6)	0.2041	6	0.4126	6
Q Tubes® 250 (N_7)	0.5934	2	0.7729	1

Table-10.evaluation and ranking of the candidate nanomaterials

Stage-3 Selection by the user

The ranking done by TOPSIS and graphical methods are slightly varied from each other. The user find out which method is the best suited for his application. Thus the nanomaterial is ranked in order of preference based on the attributes selected. However, before a final decision is taken to purchase a new nanomaterial, the following factors come into picture:- (1) Economic considerations, (2) Availability, (3) Management constraints are corporate policies, (4) SWOT analysis, (by Keeping the short term and long term objectives in mind), comprehensive SWOT analysis by the designer, device manufacturer and R & D organizations helps in the development of creative and innovative nanodevices, (5) International market policies, which were not previously considered in coding and evaluation. Even if the above consideration, say, economic considerations, does not allow the user to buy the top ranked nanomaterial, the user knows which one is better accordingly to their need and go for the next choice. For example, 2nd and 3rd ranked nanomaterial costing the same, but as our result indicates, the 2nd ranked nanomaterial performs better in other aspects even though their price is same.

Step-by-step procedure for optimum selection of nanomaterial

Step-1:- Decide about the aims and objective for which nanomaterial is to be used as per the considered application.

Step-2:-Identify all the possible alternative nanomaterial available in the literature and global market.

Step-3:-Use cause and effect diagram to find out different classes/groups of attributes/properties/characteristics and different attributes in identified classes.

Step-4:-Develop an n-digit coding scheme for characterization/specification of nanomaterial for storage and retrieval in the computer. It helps in in-depth understanding of nanomaterial.

Step-5:-Carry out elimination search to reduce the large list of alternatives nanomaterial to a manageable list of nanomaterial as per the considered application.

Step-6:-Select TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) as attribute based evaluation procedure for this small list of alternatives for ranking.

Step-7:-After evaluation, rank the candidate nanomaterial in order of preference for given application.

Step-8:- Final selection by the user from this ranked list based on external considerations or either by SWOT analysis by keeping in mind short or long term strategy.

V. RESULTS AND DISCUSSION

Results: An illustrative problem of ranking and selection of nanomaterial is solved using TOPSIS method. The problem considers seven candidate nanomaterial and five attributes (table 8**)**. In this example, specific surface area, aspect ratio of nanomaterial is beneficial attributes and the remaining 3 attributes are non-beneficial attributes as per the considered application. By applying the 3-stage procedure for optimum selection and ranking of nanomaterial results are obtained. The results for the selection and ranking of nanomaterial are obtained via, TOPSIS method and Graphical methods and it is compared with each other for selection of nanomaterial for given application (table10**)**.The evaluation and ranking of the nanomaterial using the novel graphical methods are done by their similarity to +ve benchmark nanomaterial. By using this, the max and min value of the target properties of the nanomaterial by considering target value is achieved in accordance to the given application.

Discussion: Attribute based characterization helps the scientists and product developers working in the area of nanotechnology to understand different nanomaterial in depth for possible research and development (R & D) applications and developing new nanoproducts. The attribute knowledgebase grows with the addition of new nanomaterial and new attributes for present and future applications.

- The effect of units and magnitudes of the attributes is normalized, Aims and objectives of R & D in the development of new methodology and nanoproducts decide the relative importance of attributes which is suitably addressed in the methodology.
- It is absolutely necessary that all the attribute information must be available in the attribute knowledgebase. Special efforts must be made by the inventors and developers of nanomaterial and nanotechnology at large.
- **MATLAB** software are used to find out the weights for different attributes for given application and suitability/goodness/proximity index C_i*for ranking purpose.
- The method is flexible enough and permits selection of optimum nanomaterial in the presence of large number of feasible nanomaterial and attributes. The method ensures that the selected (optimum) nanomaterial is closest to the hypothetical best nanomaterial and farthest from hypothetical worst nanomaterial.

TOPSIS method ranked the short-listed seven nanomaterial as $N_3 > N_7 > N_4 > N_2 > N_5 > N_6 > N_1$, whereas graphical method suggests the ranking as $N_7 > N_3 > N_4 > N_5 > N_2 > N_6 > N_1$. It is recommended that nanomaterial N_3, i.e. QGraphene® - 50 is the first choice, and Q Tubes® 250, QSI-Nano® Silver, NanoXact™ AU Nanoparticle, AgNW60, NanoPore™ HP-150, and AgNW115 are placed in the second, third, fourth, fifth, sixth and seventh choices, respectively. Whereas, Graphical method suggests nanomaterial alternative N_7, i.e. Q Tubes® 250 is the first choice, QGraphene® - 50, QSI-Nano® Silver, are second and third choice, , AgNW60 , NanoXact™ AU Nanoparticle are placed in fourth and fifth choice and NanoPore™ HP-150 and AgNW115 placed in sixth and seventh place respectively. Both the methods suggest that the alternative N_1, i.e. AgNW115 is the last choice. According to the TOPSIS method Q Graphene® - 50 is the best alternative because the maximum value of specific surface area and aspect ratio is achieved by using this standard nanomaterial, so that this alternative is selected as most appropriate for the considered application.

VI. Conclusions

The paper presents nanomaterial selection procedure based on the Multiple Attribute Decision Making (MADM) approach, which is a concept used not so far for the purpose. It identifies the various attributes which need to be considered for the optimum evaluation and selection of nanomaterial. It provides a coding system for nanomaterial which depicts the various attributes. It recognizes the need, processes the information, and finds the relative importance of attributes for a given application without which inter-attributes comparison is not possible. It presents the results of the information processing in terms of a merit value, which is used to rank the nanomaterial in the order of their suitability for the given application.

The contributions of the work are summarized as:-

1. The method is especially suitable for generating data of nanomaterial available in the market and their subsequent retrieval. It provides a coding scheme to produce an electronic database of globally available nanomaterial.

2. The data is helpful to all sort of peoples related to nanomaterial manufacturer, designers, and users to maintenance personnel. It is also helps to improve the overall productivity of the organization by getting the best possible solution in a minimum possible time.

3. By identifying 96 attributes of the nanomaterial, an attempt has been made to codify most of the nanomaterial characteristics, which define the nanomaterial precisely and accurately. The coding scheme is illustrated with example.

4. Evaluation and ranking based on the mathematical and graphical approaches along with the illustrative examples are given.

5. MATLAB program is developed to implement proposed methodology with the help of an illustrative example.

6. TOPSIS method ensures that the selected optimum nanomaterial is closest to positive benchmark (best) solution and farthest from negative benchmark (worst) solution.

The methodology is illustrated in this paper for optimum selection of nanomaterial. Work is in progress to select optimally different subsystems in an integrated way in the overall nanotechnology project. The present work is being extended as future work for sensitivity analysis of attribute(s) - one at a time and in combination is an important issue for R & D of new nanomaterial and feasibility analysis of different nanomaterial for various applications as potential candidates.

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