Proceedings of 4th RIT Post Graduates Conference (RIT PG Con-18)
NOVATEUR PUBLICATIONS
JournalNX- A Multidisciplinary Peer Reviewed Journal (ISSN No:2581-4230)
April, 13th, 2018

SELECTION OF CATALYST MATERIAL FOR CATALYTIC CONVERTER BY USING WEIGHTED PROPERTY INDEX METHOD

Vidyasagar B. Maske
Rajarambapu Institute of Technology
Rajaramnagar, India
vidyasagarmaske@gmail.com

Sanjay T. Satpute
Rajarambapu Institute of Technology
Rajaramnagar, India
sanjay.satpute@ritindia.edu

Abstract— Catalytic converter is an important after treatment device for emission control in automobiles. Conversion rate of harmful exhaust emission gas in catalytic converter and its efficiency is directly related to design factors of converters such as catalyst materials, wash coat material, substrate material, substrate design and other design factors. Amongst all the factors selection of material for catalyst is considered to be the most important as it deals with exhaust molecules to form nontoxic exhaust emission like nitrogen, carbon dioxide, hydrogen and also it can result in reduction of back pressure by design optimization. Various materials have been used as catalyst for catalytic converter which ranges from precious metals like platinum, palladium and rhodium etc. to non-noble metals such as cobalt, zirconium etc. The selection of materials has greater significance in catalytic converter design because of the vast activity in material science. Therefore, the range of material available to engineers are much larger than ever before. To accomplish better performance at lower price requires as more rational process for material selection. This paper deals with the recent material selection methodology by using weighted property index method (WPIM) to select material for catalytic converter. The emission performance of a converter is primarily function of properties of the catalyst. So, in case of selecting catalytic material, there are different parameters that one might consider for catalyst selection. However, in this method five different important catalytic properties are selected as required characteristic which includes valency, density, ionization energy, thermal conductivity, and thermal expansion. They were optimized using WPIM. The results of the present paper on WPIM gives best material selection for converter. The selected material is again optimized by using cost per unit method and result shows best material by considering cost also for catalytic converter which is also mentioned in other previous research paper.

Keywords— Emission, Catalytic Converter, Catalyst Material, Catalytic properties, Weighted property index method.

I. INTRODUCTION

Air pollution from automobile sources in major cities around the world has become a major concern for urban air quality, emissions from engines contains toxic gases such as carbon monoxide (CO), nitrogen oxides (NO) and unburned hydrocarbons (HC) along with longer amounts of partially oxidized organic compounds. In order to control the emissions from automobiles, sophisticated new engine technologies are introduced and also to meet stringent emission standards it has become a compulsion to introduce in vehicle. Thus, there is a direct need of treating engine pollutants gases and because of which the catalytic converter systems are being introduced in automobiles. Previously, Platinum Group Metals (PGM) have been used as a catalyst in commercially available catalytic convertors in which high surface area alumina has been used as washcoat and ceramic or metallic substrate for support. However, due to erosion and deterioration caused by thermal and mechanical stresses during longer operational periods, PGMs are emitted in the environment. Increasing concentration of PGMs in environment due to use of PGM based catalytic converter, and also those are dangerous to health which has been found in different studies [1]. Now a day, at large scale research has been carried out by using different materials with different treatment for considering the environmental issues. Ramirez Garza et al., [11] have used Mordenite-supported bimetallic (Cu-Ag) as catalysts and these were prepared for NO reduction. The maximum catalytic activity was shown for Cu (1.5) and Ag (1.5) with 70 % catalytic conversion at 380 °C. Bouck, R.M. et al., [12] have used the Cobalt-alumina as catalyst and it has been prepared by sol gel method. Preliminary catalytic tests showed that pre-heating Co-Al aerogels to 750 °C improves catalytic performance. Material pre-heated at 750 °C shows the improved catalytic conversion efficiency for CO, HC, and NOx as 89%, 9% and 80% at 740, 750 and 750 °C respectively. R. M. Bagus Irawan et al., [13] have carried out research by using Manganese Coated Copper catalyst. The substrate with different cell density of 5, 10 and 15 had been used in this research out. The maximum catalytic oxidation of CO was observed to be 79.6 %. Thus, result shows that cell density as well as material Manganese which is coated with copper has effect on catalytic activity. Femina Patel et al., 2013 [14] have conducted experiment by using Perovskite type catalysts $La_{1-x}Sr_xCoO_3$ (x=0, 0.2) composition synthesized by co precipitation method which were tested for carbon monoxide (CO) oxidation. The prepared perovskite samples were characterized. Result shows that strontium substitution in $LaCoO_3$ is responsible for enhanced CO oxidation activity due to easy reduction of transition metal and oxygen desorption properties. $La_{0.8}Sr_{0.2}CoO_3$ exhibited higher activity for CO conversion than $LaCoO_3$. 100% CO oxidation at 268°C was achieved with this catalyst. Thus, the catalyst selection has become an important stage in designing catalytic converter.

A large number of available alternative materials, having complex relationships with various selection parameters (criteria), make the material selection process a challenging task. Selection of the most suitable material involves the study of a large number of factors, like mechanical, electrical and physical properties, and cost considerations of the materials. In case of mechanical design, the mechanical properties of the materials are given the top priorities [2]. The significance of materials selection in design is greater than before. The vast activity in materials science worldwide has formed new materials and focused concentration on the contest between six groups of materials viz. metals, polymers, elastomers, ceramics, glasses, and composites. Therefore, the range of materials available to the engineer is much larger than ever before. To accomplish better performance at a lower price requires a more rational process for materials selection [3]. A design demands requires a certain profile of important properties and to start with the full menu of materials in mind. There is need to identify the desired attribute profile by examining the design requirements and to identify the constraints that they impose on material choice. The immensely wide choice is narrowed, by screening-out the materials that cannot meet the constraints. Further, narrowing is achieved by ranking the candidates by their ability to maximize performance. Criteria for screening and ranking are derived from the design requirements for a component by an analysis of function, constraints, objectives, and free variables [4]. There are different methods by which material can be selected as per above stated criteria of which some are discussed here.

II. Material Selection Methodologies

In the product development, material is a key aspect of product and so the method and process used to select the material. Also, it plays an important role in designing process. Thus, there are number of selection methods which are being used and thoughts in academic. From all those methods, the cost per unit method is the one which is suitable for initial screening in applications where one property stands out as the most critical service requirement [5]. Value Engineering is the another method which is an systematic application of recognized techniques by multi-disciplined teams that identifies the function of a product or service; establishes a worth for that function, generates alternatives through the use of creative thinking and provides the needed functions, reliably, at the lowest overall cost, thus, it is a systematic method to improve the "value" of goods or products and services by using an examination of function [6]. Weighted property index method is used when material is need to be selected by optimization of more than one properties. The typical approximation is to allocate a weighting factor to each material condition or property, relying on its significance [7]. This method is used to select material in this study. In order to select the material using this particular method, for the application of catalytic converter it is required to know the important properties that can be physical or chemical properties which is described in further part. Thus, this method seems to be most appropriate for material selection compare to other methods.

III. Material Properties

Three Way Catalytic Converter (TWC) deals with the exhaust gas molecules to form nonhazardous emissions like Nitrogen, Carbon Dioxide, Hydrogen Dioxide and can also be aimed at reduction in back pressure by design optimization. Numbers of materials have been used as catalyst from precious metals like Platinum (Pt), Rhodium (Rd) to Non-Noble Metal Catalyst like Copper, Cobalt, and Zirconium etc. The emission performance of a converter is primarily function of properties of the catalyst. The ionization energy (IE) is the chemical property which is qualitatively defined as the amount of energy required to remove the most loosely bound electron, the valence electron and it is inversely proportional to catalytic activity. So, it must be less in order to get large activity [8]. Valence electron is an outer shell electron that is associated with an atom, and that can participate in the formation of chemical bond, if the outer shell is not closed. The presence of valence electron can determine the element chemical properties, such as it valence. The density, or more precisely, the volumetric mass density, of a substance is its mass per unit. Catalyst quantities are typically specified commercially on the basis of volume and bulk density. Particle density is often used in calculating Thiele modulus for a mass-based rate constant and converting rate between volume and mass bases [9]. Thermal conductivity is the property of a material to conduct heat. It is evaluated primarily in terms of Fourier's Law for heat conduction. Heat transfer occurs at a lower rate across materials of low thermal conductivity than across materials of high thermal conductivity. Correspondingly, materials of high thermal conductivity are widely used in heat sink applications and materials of low thermal conductivity are used as thermal insulation. The thermal conductivity of a material may depend on temperature. Thermal expansion is the physical property of material in which the matter changes its shape, area and volume in response to a change in temperature.

IV. Material selection by WPIM

In this paper, material has been selected by weighted property index method and its step wise process is described below. Initially, screening of transitions elements has been considered for those material which are having catalytic properties. As these elements are used for other catalytic applications, noble metals from the literature has been selected such as Ruthenium (Ru), Rhodium (Rh), Palladium (Pd), Silver (Ag), Osmium (Os), Rhenium (Re), Iridium (Ir), Platinum (Pt), Gold (Au) and Copper (Cu).

A. Catalytic properties of noble metals

Catalytic properties of noble materials are listed separately from which chemical properties such as valency (V), oxidation state, ionization energy (IE). Physical properties are density (ρ), melting point (MP), boiling point (BP), thermal conductivity (K), coefficient of thermal expansion (TE) and along with their particular element cost for ten grams.

TABLE 1. CHEMICAL PROPERTIES OF NOBLE METALS [10]

Sr. No.	Elements	Valency	Oxidation state	Ionization energy (KJ/mol)
1	Ru	8	3,4	710.2
2	Rh	6	3	719.7
3	Pd	4	2,4	804.4
4	Ag	4	2,4	731
5	Re	7	4	760
6	Os	8	4	840
7	Ir	8	3,4	880
8	Pt	6	2,4	870
9	Au	5	3	890.1
10	Cu	4	2	745.5

TABLE 2. PHYSICAL PROPERTIES OF NOBLE METALS [10]

Elements	**MP (K)**	**BP (K)**	**ρ (Kg/m³)**	**K (W/mK)**	**TE (µm/(m·K) (at 25 °C))**	**Cost/10 gram (Rs.)**
Ru	2607	4423	12370	120	6.4	2700
Rh	2237	3968	12450	150	8.2	36000
Pd	1828.05	3236	12023	72	11.8	21038.5
Ag	1234.93	2435	10490	430	18.9	342.93
Re	3459	5869	21020	48	6.2	4000
Os	3306	5285	22610	88	5.1	12000
Ir	2739	4701	22650	150	6.4	25000
Pt	2041.4	4098	21090	72	8.8	29000
Au	1337.33	3129	19300	320	14.2	26745
Cu	1357.77	3200	8920	400	16.5	152

B. Digital Logic Method

In this stage, each property is weighted and factor is assigned to each element according to their weightage as given in table 3. Total five properties have been selected for this catalyst material selection those are density (δ), valency (V), thermal conductivity (K), Ionization energy (IE), and thermal expansion (TE). The total number of possible decisions is calculated as N = n (n - 1) / 2, where n is the number of properties consideration.

$$\therefore N = \frac{n(n-1)}{2}$$

$$= \frac{5(5-1)}{2} = 10$$

There are total ten possibilities which can be interrelated as shown in Table 3. Thus, the weighting factor has been calculated and it has been assigned to each property. The summation of all should be equal to 1.

TABLE 3. DETERMINATION OF RELATIVE IMPORTANCE OF MATERIAL PROPERTIES USING DIGITAL LOGIC METHOD.

			Possibilities											
Sr. No.	**Properties**		**1-2**	**1-3**	**1-4**	**1-5**	**2-3**	**2-4**	**2-5**	**3-4**	**3-5**	**4-5**	**+ ve Decisions**	**Weighting factor**
			1	2	3	4	5	6	7	8	9	10		α
1	ρ	1	1	0	0	1							2	0.2
2	V	2	0				1	0	1				2	0.2
3	K	3		1			0			1	1		3	0.3
4	IE	4			1			1		0		0	2	0.2
5	TE	5				0			0		0	1	1	0.1
												Σ	10	1

C. Performance Index

The weighted properties index has the disadvantage of having to combine properties with dissimilar units thus, it has been stabilizing by using a scaling factor [7]. The scaling factor for valency, density and thermal conductivity for which higher value is required, is calculated by using equation (1) as,

$$\therefore \beta = \frac{\text{numerical value of property}}{\text{largest value}} \times (100) \quad \text{........ (1)}$$

Sample calculation for βmax valency of rhodium (Rh),

$$\therefore \beta = \frac{6}{8} \times 100 = 75$$

For properties like ionization energy and thermal expansion for which a low value is best as given in equation (2), the scale factor is defined as:

$$\therefore \beta = \frac{\text{lowest value in list}}{\text{numerical value of property}} \times (100) \quad \text{........ (2)}$$

Sample calculation of βlow thermal expansion for ruthenium (Rh) as,

$$\therefore \beta = \frac{5.1}{6.4} \times 100 = 79.68$$

The values of β for all properties has been calculated and multiplied with their respective property weighting factor. Then the summation of Σαβ has been calculated to find the weighted property index for each element as given in Table 4.

Thus, the sample calculation for WPI as shown in equation (3) for ruthenium is given as,

$\gamma = \sum_{i=1}^{n} \beta_i W_i$ ……… (3)

$$\therefore \gamma = (0.2 \times 100) + (0.2 \times 54.6) + (0.3 \times 30) + (0.1 \times 79.68) + (0.2 \times 100) = 69.891478$$

Thus, from the above table the value of property index method has been calculated for each metal and the metal having highest WPI can be selected as the suitable material for particular application, but it is without considering the cost of metals. In this case, Iridium is found to be the suitable as per our priority for properties using weighted property index method. Thus, by considering cost it has given in next stage as cost also an important factor.

D. Cost Consideration

Cost can be considered as one of the properties and now a day it has become a need to consider the cost while selecting or designing material. However, if there is a large number of properties to consider, the importance of cost may be emphasized by considering it separately as a modifier to the material performance index γ. In the cases where the material is used for space filling, cost can be introduced on a per-unit-volume basis as given in Table 5. A figure of merit γ' for the material can then be defined as from equation (4),

$\gamma' = \frac{\gamma}{C\delta}$ ……. (4)

Where, C = total cost of material per unit weight, δ = density of material

Thus, from the weighted property index chart considering cost per unit volume, the performance index has been calculated, and it can be observed that Copper has the highest performance index value as 0.051. Hence, Copper metal can be selected as a catalytic material for the three-way catalytic converter by considering those selected property as per the decided priority in this method and also prioritizing the cost. We can change the priority and properties as per the experience having about properties and alter the sequence and priority as per our requirements.

TABLE 4. PERFORMANCE INDEX CHART

	α	α = 0.2			α = 0.2			α = 0.3			α = 0.1			α = 0.2		Weighted Property Index (WPI)
Elem-ent	V	β Max	Σαβ	δ × 103	β Max	Σαβ	K	β Max	Σαβ	TE	β Low	Σαβ	IE	β Low	Σαβ	(γ)
Ru	8	100	20	12.37	54.6	10.92	120	30	9	6.4	79.68	7.96	710.2	100	20	67.891
Rh	6	75	15	12.45	54.966	10.99	150	37.5	11.25	8.2	62.19	6.21	719.7	98.68	19.736	63.198
Pd	4	50	10	12.02	53.081	10.61	72	18	5.4	11.8	43.22	4.32	804.4	88.289	17.658	47.996
Ag	4	50	10	10.49	46.313	9.262	430	107.5	32.25	18.9	26.98	2.69	731	97.155	19.431	73.642
Re	7	87.5	17.5	21.02	92.803	18.56	48	12	3.6	6.2	82.25	8.22	760	93.447	18.689	66.575
Os	8	100	20	22.61	99.823	19.96	88	22	6.6	5.1	100	10	840	84.548	16.91	73.474
Ir	8	100	20	22.65	100	20	150	37.5	11.25	6.4	79.68	7.96	880	80.705	16.141	75.359
Pt	6	75	15	21.09	93.112	18.62	72	18	5.4	8.8	57.95	5.79	870	81.632	16.326	61.144
Au	5	62.5	12.5	19.30	85.209	17.04	320	80	24	14.2	35.91	3.59	890.1	79.789	15.958	73.091
Cu	4	50	10	8.92	39.381	7.876	400	100	30	16.5	30.90	3.09	745.5	95.265	19.053	70.020

TABLE 5. PERFORMANCE INDEX PER UNIT COST PER UNIT VOLUME

	Cost/10 gram		WPI Considering cost per unit volume (γ')
Symbol	C	$\delta \times C$	$\frac{\gamma}{C\delta}$
Ru	2700	33399	0.00203274
Rh	36000	448200	0.000141006
Pd	21038.5	252945.8855	0.000189749
Ag	342.93	3597.3357	0.020471268
Re	4000	84080	0.000791817
Os	12000	271320	0.000270803
Ir	25000	566250	0.000133085
Pt	29000	611610	9.99729E-05
Au	26745	516178.5	0.000141601
Cu	152	1355.84	**0.051643463**

V. VALIDATION OF RESULT

The outcomes of this method suggest that copper would be the better material considering its given properties and also the cost as important one. From the literature it seems that copper shows the better result for the requirements and its oxidation and reduction results are satisfactory. Ghosh et al. [15] have worked on copper and they have achieved 85 % NOx, 72 % CO and HC as conversion efficiencies. Also, Irawan R. B et al. [13] have carried out work on bimetallic component using copper as main ingredient in which they have significantly reduced CO emission. Thus, from the literature, it has been seen that copper can work as the best material for catalytic converter and the WPIM method results seem to be the expected as per our requirements.

VI. CONCLUSION

Material selection is an important aspect in the catalytic converter, so WPIM selection methodology has been demonstrated by selecting noble metal for catalytic converter. In this study, material has been selected primarily by initial screening and then by using digital logic method by considering important catalytic properties. Cost has also been considered so as to make material selection as cost effective by using cost per unit volume. The calculated weighted property index considering cost shows that copper is appropriate metal for catalytic converter in noble metals for the decided priority and the selected properties. Thus, as per our requirement, preference and economical condition we can select the material by using WPIM method and from the literature it has seen that copper shows better catalytic activity. The actual or the typical catalyst selection way differ from the industrial way, so the accuracy of this method is somewhat less than actual one but then also it seems to be effective one for catalytic material selection.

REFERENCES

[1] Waleed Ahmad, Tayyaba Noor, Muhammad Zeeshan, "Effect of synthesis route on catalytic properties and performance of Co3O4/TiO2 for carbon monoxide and hydrocarbon oxidation under real engine operating conditions", Catalysis Communications 89 (2017) 19–24.

[2] Chatterjee, P., Athawale, V.M. and Chakraborty, S., 2009. Selection of materials using compromise ranking and outranking methods. Materials & Design, 30(10), pp.4043-4053.

[3] Findik, F. and Turan, K., 2012. Materials selection for lighter wagon design with a weighted property index method. Materials & Design, 37, pp.470-477.

[4] Ashby, M.F., 1993. Criteria for selecting the components of composites. Acta metallurgica et materialia, 41(5), pp.1313-1335.

[5] Maleque, M. and Sarker, D., 2010. Materials selection of a bicycle frame using cost per unit property and digital logic methods. International Journal of Mechanical and Materials Engineering, 5(1), pp.95-100.

[6] Sharma, A., Srivastava, H. and Belokar, R.M., 2011. A case study analysis through the implementation of Value engineering. International Journal of Engineering Science and Technology, 3(3).

[7] Findik, F. and Turan, K., 2012. Materials selection for lighter wagon design with a weighted property index method. Materials & Design, 37, pp.470-477.

[8] Lee, E.H., 1974. Iron oxide catalysts for dehydrogenation of ethylbenzene in the presence of steam. Catalysis Reviews, 8(1), pp.285-305.

[9] Bartholomew, C.H. and Farrauto, R.J., 2011. Fundamentals of industrial catalytic processes. John Wiley & Sons.

[10] Dayah, Michael. Ptable: The Interactive Periodic Table. 1 Oct. 1997. Web. 31 Mar 2018 <https://ptable.com>.

[11] Ramírez-Garza, R.E., Rodríguez-Iznaga, I., Simakov, A., Farías, M.H. and Castillón-Barraza, F.F., 2018. Cu-Ag/mordenite catalysts for NO reduction: Effect of silver on catalytic activity and hydrothermal stability. Materials Research Bulletin, 97, pp.369-378.

[12] Bouck, R.M., Anderson, A.M., Prasad, C., Hagerman, M.E. and Carroll, M.K., 2016. Cobalt-alumina sol gels: Effects of heat treatment on structure and catalytic ability. Journal of Non-Crystalline Solids, 453, pp.94-102.

[13] Irawan, R.B., Purwanto, P. and Hadiyanto, H., 2015. Optimum Design of Manganese-Coated Copper Catalytic Converter to Reduce Carbon Monoxide Emissions on Gasoline Motor. Procedia Environmental Sciences, 23, pp.86-92.

[14] Patel, F. and Patel, S., 2013. La1-xSrxCoO3 (x= 0, 0.2) perovskites type catalyst for carbon monoxide emission control from auto-exhaust. Procedia Engineering, 51, pp.324-329.

[15] Ghosh, B.B., Santra, P.K., Ghosh, P.P., Banerjee, T., Ghosh, A. and Ramanujam, S., 2001. Catalytic reduction of SI engine emissions using Cu-ion exchange ZSM-5 (No. 2001-26-0013). SAE Technical Paper.