

Selecting the Best Material for Hydrogen Storage Using the Analytical Hierarchical Process

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Abstract

Hydrogen is becoming more important as a source of energy for many applications. Hydrogen storage is a challenge task in developing this technology. There are many methods for hydrogen storage. The most common method to store hydrogen is complex hydrides. In this study, the analytical hierarchical process (AHP) is used to select the best material for hydrogen storage device. The model is built using four criteria, including: mechanical properties, physical properties, chemical properties and cost. LiBH₄, NaAlH₄, LiNH₂, Mg₄NiPd, KAlH₄, Mg (AlH₄), Li₃AlH₆, Na₂LiAlH₆ were used as alternatives to select among them. The results show that Mg₄NiPd is the best material. Both inconsistency and sensitivity analysis were done and showed that model is robust.

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Keywords: Analytical Hierarchical Process (AHP), Material selection, Hydrogen storage, Complex hydride

Nomenclature

AHP	Analytical Hierarchy Process	MADM	Multiple Attribute Decision-Making
AR	Average Ratio	MCDM	Multi-Criteria-Decision-Making
CR	Consistency Ratio	MODM	Multiple Objective Decision Making
II	Inconsistency Index	RI	Random Consistency Index

1. Introduction

Hydrogen gas is important for several reasons. Hydrogen is considered to be one of the most promising fuels for the future. It enters into a large number of chemical and oil industries. Hydrogen is a reducing agent for mineral elements from their ores; it is used in many physical and engineering applications, and hydrogen gas is used with nitrogen gas to detect the precise leakage in power plants and in multiple industries [1-5]. Hydrogen is an alternative future ecofriendly energy resource [6-14]. Hydrogen can mainly be stored in three different ways; as a compressed gas, liquefied or as a solid either by adsorption, absorption or reacting with different materials. Typically, small amount of gas occupied large volume hence need large tanks to store, and low

temperature to keep the gas dense or liquid. However, several studies have reported the ways of getting the highest volumetric density of hydrogen in quite small volume by packing hydrogen as close as possible [e.g. 10]. The challenge is to study the way of interaction of hydrogen with other elements to get the best hydrogen capacity of charge and discharge with good stability. The main parameters that need to be optimized to get the best storage capacity of hydrogen are; temperature, pressure, reacting with hydrogen and cost [6-17].

Complex hydride-forming materials are the most common methods to store hydrogen, due to their high storage density and safe. Mg-based alloys give the highest hydrogen capacity at room temperature due to its low hydrogen binding energy [16].

The selection of a material for hydrogen storage purpose is a long-lasting and costly process. Approximately always more than one material is suitable for hydrogen storage, and the final selection is a compromise that brings some advantages as well as disadvantages. The aim of this work is to use multiple criteria decision making (MCDM) to choose best material and method to store hydrogen at lower cost. Most researchers have studied hydrogen storage in practice, but in this research it will try to find the best material to store hydrogen using AHP model based on the following criteria. The following alternatives (LiBH₄, NaAlH₄, LiNH₂, Mg₄NiPd, KAlH₄, Mg(AlH₄), Li₃AlH₆, Na₂LiAlH₆) have been used in this work.

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2. Hydrogen Storage Methods

Storage of hydrogen is considered a challenge because it is limited due to the low density of hydrogen hence higher occupied volume which makes it difficult to store and need a huge containers. To date, a high focus has been given to develop an effective, safe and inexpensive tank system to store hydrogen especially for vehicles. Hydrogen can be stored in several ways; high-pressure tanks, cryogenic tanks as liquid hydrogen, adsorbed on material's surface, absorption, chemically bonded and oxidation of metals with water [e.g. 17]. Other studies found that the amount of hydrogen which could be stored is higher in high-pressure metal hydrate tank in comparison with high-pressure tank and low-pressure metal hydrate tank [18]. However, mechanical storage like compression and liquefaction are very expensive and need high energy [19].

Moreover, nanomaterials could be promising technology to store hydrogen, which provide huge surface area in quite small volume. For example, β -Co(OH)₂ nanowafers and nanohexagons provided an excellent storage capacity of hydrogen 265.9, 215.7 mAh/g at room temperature, respectively also showed a very good stability [20]. In addition, CuO/Al₂O₃ nanocomposites [21], layered FeMo₄S₆ nanosheets ([22], zirconia-reduced graphene oxide (ZrO₂-rGO) nanocomposite [23], different alloys [24] and hydride compounds [25] also exhibit a good capacity of hydrogen storage.

The addition of small amount of oxygen (1000 ppm) to Mg-based materials improves hydrogen storage capacity and adsorption/desorption kinetics at high temperature, and due to that the crystallization structure is improved [26].

Reversible capacity and cycling stability of hydrogen in carbon-based nanoporous materials could be improved by the addition of doping atoms such as Lithium under ambient temperature and pressure [27]. Moreover, another study [28], studied the effect of nitrogen-doping atoms in three different carbon nanostructure. According to the results, nitrogen-doped carbon nanotubes presented the highest hydrogen storage capacity.

Complex hydrides, LiBH₄, which contain 18 mass% of hydrogen, up to 13.5 mas% is liberated with SiO₂ catalyst at different steps and temperature regimes [29]

3. 3 MATERIAL SELECTING METHODS

Materials choosing methods can classify into two main sets, namely, MCDM methods and Optimization methods. The MCDM methods can be either multiple objective decision making (MODM) or multiple attribute decision making (MADM) approaches. There are several methods in each of the above categories. Each technique has its own characteristics and the methods can combine with each other or fuzzy-logic methods [30]. In this work, the analytical hierarchy process (AHP) has been used. It has been used extensively world-wide because of its simplicity, ease of use, and great flexibility. AHP has been applied, and then the sensitivity analysis has been

performed to increase the confidence in the choice of material [31-35]. AHP method has been used in this work in order to find out the relative importance of different attribute with respect to the objective in material selection.

4. Methodology and Results

A five-step method to select the best material in complex hydrides for hydrogen storage using AHP model has been proposed. This process has been achieved by the aid of special software called (Expert choice)TM[36-37]. Figure (1) shows the flow chart that describes the methodology of the work. The following is a pseudo code of the algorithm of the main program: **Algorithm:**

4.1. Initialization:

Step 1: Set up decision hierarchy by selecting all possible criteria and alternatives.

Step 2: Make pairwise comparisons of attributes and alternatives to determine the relative importance of attributes, and compare how well the alternatives perform on the different attributes.

Step 3: Transform comparisons into weights and check consistency.

Step 4: Use weights to obtain scores for alternatives, and the alternative that has the highest score will be the best alternative.

Step 5: Carry out sensitivity analysis.

4.1.1. Step one: Set up decision hierarchy.

The decision hierarchy is the basic step in AHP. It is established by selecting many of the possible criteria and alternatives based on literatures. According to literature survey, the hierarchy was built using four criteria, including: mechanical properties, physical properties, chemical properties and cost. LiBH₄, NaAlH₄, LiNH₂, Mg₄NiPd, KAlH₄, Mg (AlH₄), Li₃AlH₆, Na₂LiAlH₆ were used as alternatives to select among them [1-16]. After determination many of the possible criteria and alternatives, the value tree that contains the objective, criteria, sub criteria, alternatives had been built. Figure (2) illustrates this value tree.

4.1.2. Step two: Make pairwise comparisons of attributes and alternatives.

The pairwise comparisons of attributes and alternatives are done at each node of the value tree and used to determine the relative importance of attributes, and compare how well the alternatives perform on the different attributes. An expert in hydrogen storage and based on long-list literatures, makes pairwise comparisons by giving a scale for each pairwise comparison. This scale is given based on strength of importance, as shown in Table (1). The output pairwise comparison matresise of this step, for each node, are shown in Table (2) and in Figures (3-7) that will be explained later.

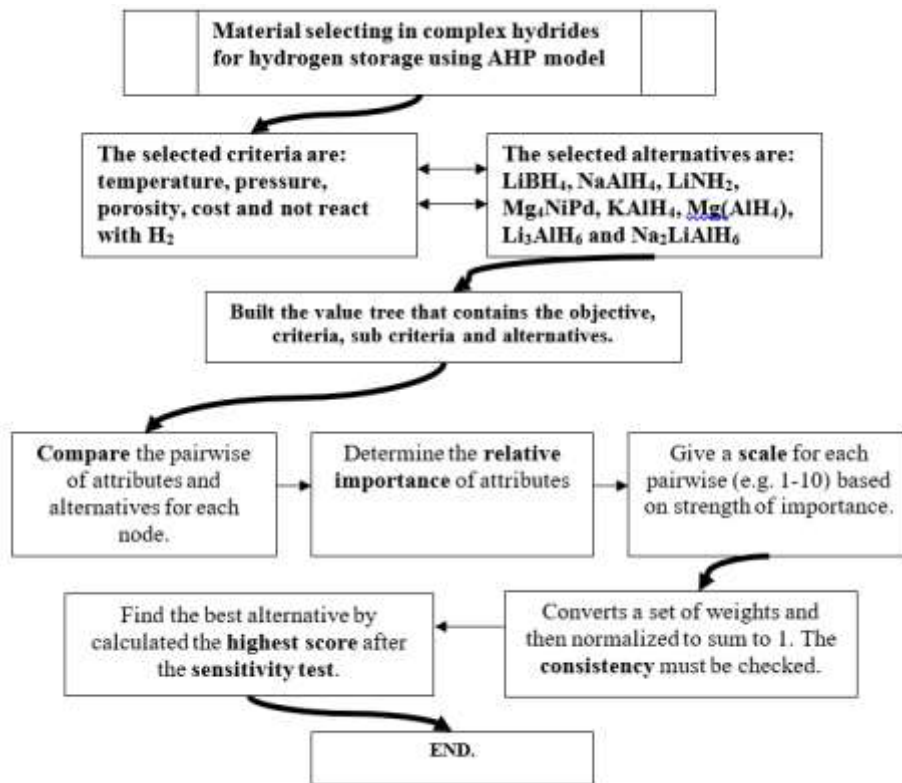


Figure 1. The flow chart of Material selection methodology based on AHP.

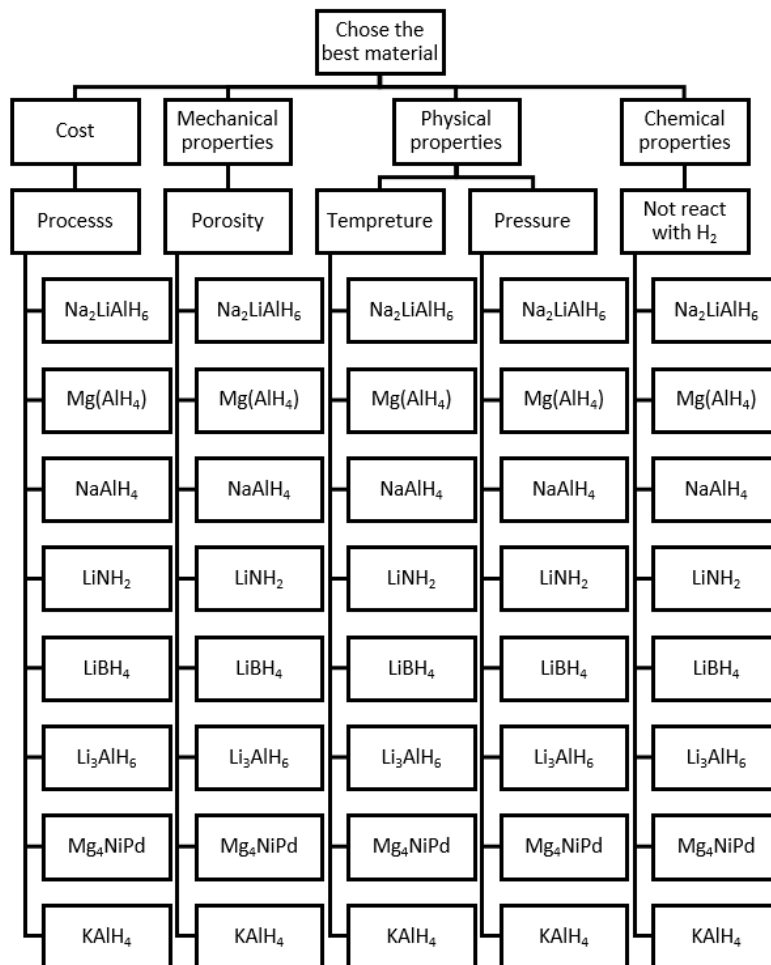


Figure 2. Value tree for alternatives of complex hydrides materials using AHP model

Table 5. The consistency final calculation of the main criteria with respect to Cost.

Material	Total weight from Table (4)	Priority from Table (3)	Total weight / Priority
LiBH ₄	1.850	0.208	8.894
NaAlH ₄	0.826	0.095	8.699
LiNH ₂	1.444	0.165	8.748
Mg ₄ NiPd	0.809	0.093	8.697
KAlH ₄	0.430	0.05	8.606
Mg(AlH ₄)	1.158	0.133	8.703
Li ₃ AlH ₆	1.505	0.172	8.750
Na ₂ LiAlH ₆	0.742	0.084	8.829
Average of (Total weight / Priority) = 8.741			
II (inconsistency index) = (8.741 – 8)/7 = 0.106			
Consistency Ratio (CR) = II/RI = 0.106 / 1.41 = 0.075			

Tables (2-5) belonged to the calculation of the main criteria with respect to Cost only. Similar calculation must be repeated for each property and the interlock relation between them must be extracted. Obviously, this is a time-consuming procedure and needing enormous efforts. This problem resolved by conducting the analysis using “Expert Choice” software that greatly facilitates this process. “Expert Choice” is decision-making software that is based on MCDM. “Expert Choice” implements AHP based on Saaty works [e.g. 36-37] and has been used for long time in many fields [38-40]. All data were entered to this user-friendly software and the results are showed in figures (3-12).

Figure (3) presents the effect of cost on selecting the material. This figure summarizes all the manual calculation that carried above and recorded in tables (2-5) and both results are identical. The right hand part of this figure is the pairwise comparison matrix built on the relative cost of each alternative materials. Note here that only half of matrix is shown as the other half are the reciprocals (i.e. $a_{ji} = 1/a_{ij}$). Note, also, that the red colour number used by the software shows inverse value. The left hand part of the figure contains a horizontal bar chart that indicates the weight of each material with respect to the cost. Accordingly, LiBH₄ is the best choice with respect to cost. This figure shows, also, the inconsistency ratio with a value of 0.08 which is acceptable as it is below 0.1.

Figure (4) offerings the effect of porosity as a mechanical properties on selecting the material. The pairwise comparison matrix built according the relative porosity of each alternative materials is shown. The horizontal bar chart indicates that LiBH₄ is the best choice again. The inconsistency ratio is 0.05 which is in the acceptable range.

Figure (5) shows the effect of temperature on selecting the material. The pairwise comparison matrix built according the effect of temperature of each alternative materials is shown. The horizontal bar chart indicates that Mg₄NiPd is the best choice in this case. The inconsistency ratio is 0.04 which is in the acceptable range.

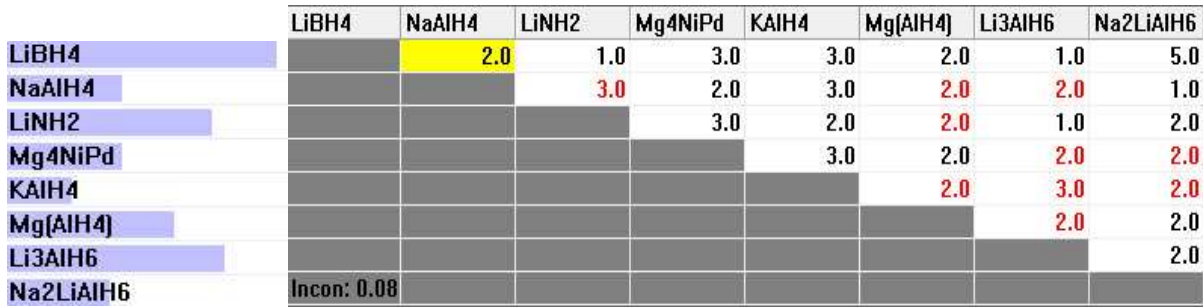


Figure 3. Pairwise comparison matrix of the main criteria with respect to Cost.

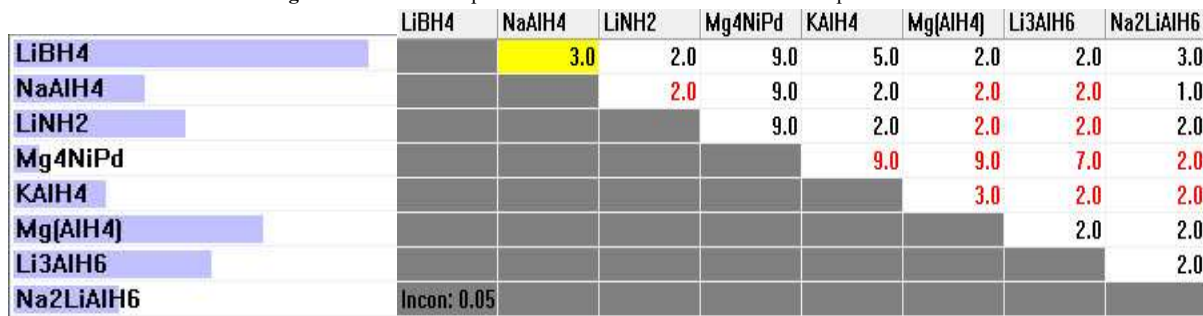


Figure 4. Pairwise comparison matrix of the main criteria with respect to Mechanical Properties/ Porosity



Figure 5. Pairwise comparison matrix of the main criteria with respect to Physical Properties/ Temperature.

Figure (6) shows the effect of pressure as another physical properties on material selection. The pairwise comparison matrix built according the effect of pressure of each alternative materials is shown. The horizontal bar chart indicates that LiBH₄ is the best choice in this case. The inconsistency ratio is 0.06 which is, also, in the acceptable range.

Figure (7) shows the effect of chemical reaction on material selection. The pairwise comparison matrix built according to the effect of chemical properties of each alternative materials is shown. The horizontal bar chart indicates that Mg₄NiPd is the best choice in this case. The inconsistency ratio is 0.05 which is, also, in the acceptable range.

4.1.4. Step four: Use weights to obtain scores for alternatives.

After calculating the weights and checking consistency for each table, we can find the best alternative by calculated the

score for each alternative and the alternative that has the highest score will be the best alternative. Figure (8) contains all results calculated from figures (3-7) after normalising (lengthly manual calculated are not shown). Each column contains a horizontal bar chart that shows the distribution of the effect of this property on the material selection. Note here that the highest value of each column is one (normalising).

Figure (9) shows the hierarchy of the criteria with the priority of each criterion and the final rank. The two physical properties (the temperature and pressure) were treated together with the ratios of (0.75:0.25). This figure shows that physical properties are the most important factors in the goal of the study with a total weight of 0.526 (52.6 %). On the other side, the process cost is the least important factor with a weight of less than 10 %. The inconsistency for this part of analysis is 0.02 that is acceptable.

	LiBH4	NaAlH4	LiNH2	Mg4NiPd	KAlH4	Mg[AlH4]	Li3AlH6	Na2LiAlH6
LiBH4		3.0	2.0	2.0	5.0	2.0	2.0	3.0
NaAlH4			2.0	3.0	3.0	2.0	5.0	1.0
LiNH2				2.0	2.0	3.0	2.0	2.0
Mg4NiPd					2.0	2.0	2.0	3.0
KAlH4						2.0	3.0	2.0
Mg[AlH4]							2.0	3.0
Li3AlH6								2.0
Na2LiAlH6	Incon: 0.06							

Figure 6. Pairwise comparison matrix of the main criteria with respect to Physical Properties/ Pressure.

	LiBH4	NaAlH4	LiNH2	Mg4NiPd	KAlH4	Mg[AlH4]	Li3AlH6	Na2LiAlH6
LiBH4		2.0	2.0	5.0	3.0	2.0	2.0	2.0
NaAlH4			2.0	3.0	2.0	3.0	1.0	1.0
LiNH2				2.0	2.0	2.0	1.0	7.0
Mg4NiPd					2.0	3.0	3.0	
KAlH4						2.0	2.0	3.0
Mg[AlH4]							2.0	2.0
Li3AlH6								2.0
Na2LiAlH6	Incon: 0.05							

Figure 7. Pairwise comparison matrix of the main criteria with respect to Chemical Properties/ Not React With H₂.

Alternative	Pairwise	Pairwise	Pairwise	Pairwise	Pairwise
	Cost Process (L: 1.000)	Mechanical Properties Porosity (L: 1.000)	Physical Properties Temperature (L: .750)	Physical Properties Pressure (L: .250)	Chemical Properties Not react with hydrogen (L: 1.000)
✓ LiBH4	1.000	1.000	161	1.000	267
✓ NaAlH4	.445	.368	308	.279	214
✓ LiNH2	.780	.407	116	.663	455
✓ Mg4NiPd	.436	.073	1.000	.667	1.000
✓ KAlH4	.233	.261	.078	.293	623
✓ Mg[AlH4]	.625	.717	.075	.420	483
✓ Li3AlH6	.013	.568	.103	.728	268
✓ Na2LiAlH6	.400	.308	.272	.272	155

Figure 8. Alternative prioritization matrix for all criteria.

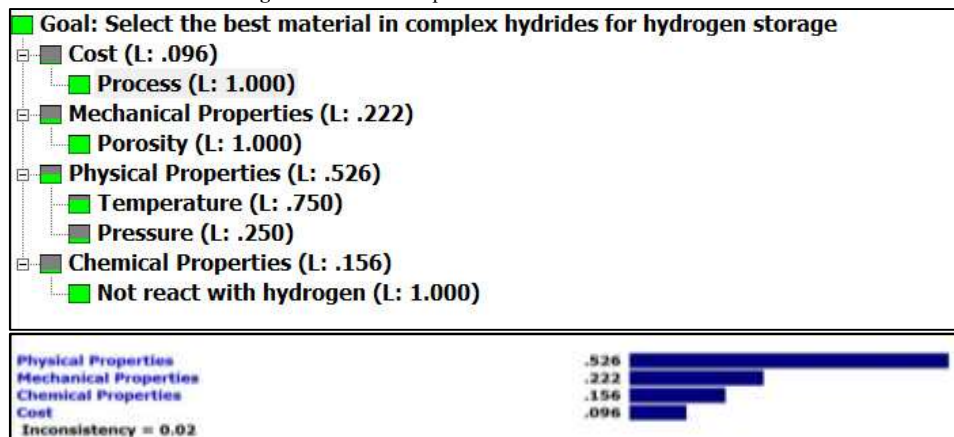


Figure 9. The hierarchy of the criteria with the priority of each criterion for alternative total weight and final rank.

4.1.5. Step five: Carry out sensitivity analysis.

The last step is the sensitivity analysis, and it is used to examine how robust the choice of an alternative is to change in the figures used in the analysis. Figure (10) shows the total weight each criteria and alternative. Figure (11), also, shows the total weight of each criteria in its left side. Whilst, the right side is a horizontal stacked bar chart that shows the decomposition of the effect of each criteria on each alternative.

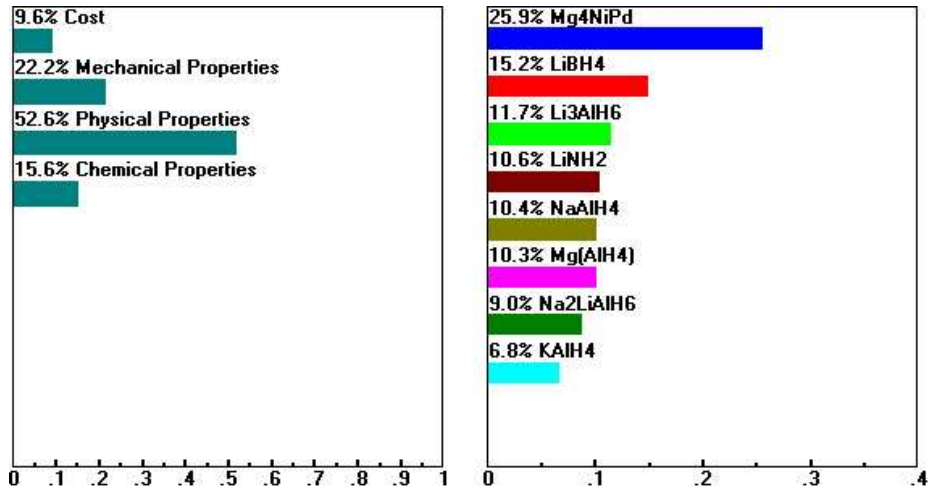


Figure 10. Total weight for each criteria and each alternative.

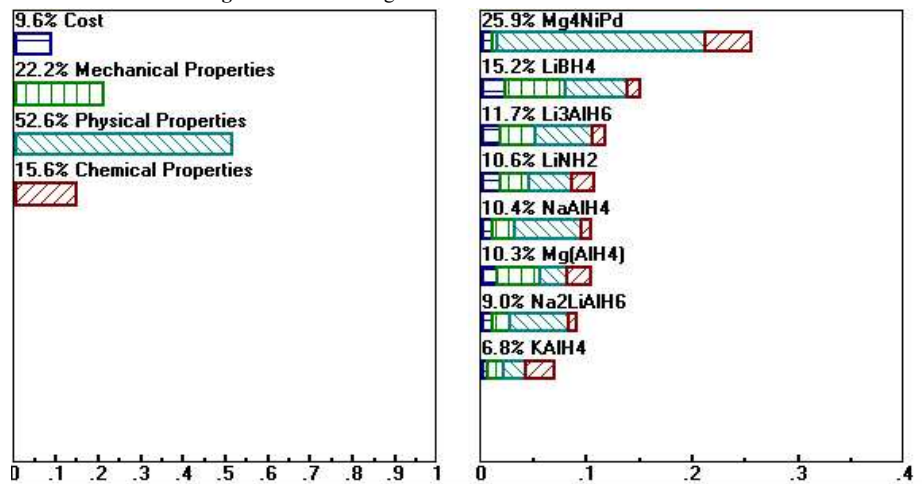


Figure 11. Total weight for each criteria (left) and effect of it on each alternative (right).

Performance Sensitivity for nodes below: Goal: Select the best material in complex hydrides for hydrogen storage

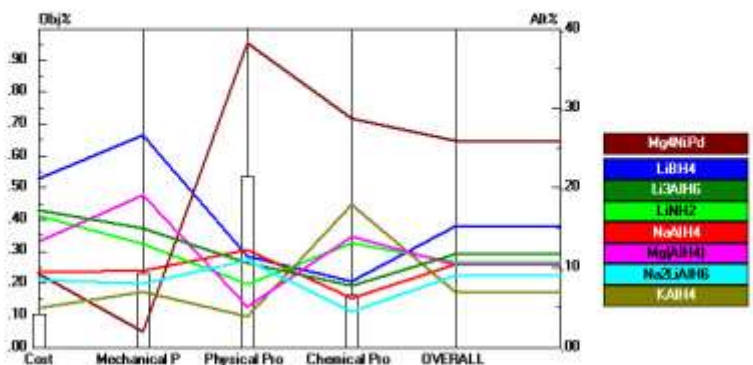


Figure 12. Performance sensitivity test with respect to the main goal.

Figure (12) shows the performance sensitivity test that confirms the acceptance level of accuracy for the analysis. This figure validates the above analysis results. The left side vertical axis belongs to the vertical bar chart that shows the final rank of the main criteria to the target goal. The right hand vertical axis belongs to multi-colour line diagrams that represents the contribution of each criteria on the selection of each alternative material.

5. Conclusions

- Complex hydride-forming materials are the most common method to store hydrogen, due to their high storage density and safe. LiBH_4 , NaAlH_4 , LiNH_2 , Mg_4NiPd , KAlH_4 , $\text{Mg}(\text{AlH}_4)_2$, Li_3AlH_6 , $\text{Na}_2\text{LiAlH}_6$ were used as alternatives to select among them.
- The model is built using four criteria including: mechanical properties, physical properties, chemical properties and cost.
- AHP is used as MCDM with the aid of special software called (Expert Choice)TM.
- The results show that the best material to store hydrogen is Mg_4NiPd .
- Physical properties were more important than other criteria as shown in the above analysis.
- Both inconsistency and sensitivity analysis were done, and showed that model is robust. All the Consistency ratios, throughout the study, had been less than 0.1 that is acceptable.
- As future work, the extension of the method to include the energy analysis when storing/releasing hydrogen could be added as some metal hydrides require cooling/heating during charging/dischARGE. More criteria and material could be considered.

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