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Choosing Thermos Chemical Storage Materials for High Temperatures Using a MCDM Methodology

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Abstract. Because of its inherent variability, intermittency, and technological and economic difficulties, currently, manufacturing waste heat is underutilized. One of the best methods for removing obstacles, lowering greenhouse gas emissions, and safeguarding the ecosystem at large is energy recovery. The process of choosing materials is crucial to the design of heat storage devices. Complex interactions between a number of variables and parameters are necessary to produce the finest candidate material for a particular application. The selection of high-temperature thermo chemical storage (TCS) materials is addressed in this research using a matrix-based multi-criteria decision-making (MCDM) approach. The Port Talbot Steelworks also utilized the suggested method to select suitable components for high temperature waste heat recovery (above 500 C). In this article, a COPRAS set theory-based multi-criteria decision-making (MCDM) model is proposed. Alternatives include MgH2, MgH2/Composite, Mg2FeH6, Mg2NiH4, MgO/Mg(OH)2, and Heat Release Temperature. Evaluation criteria also include Reaction Enthalpy, Volumetric Energy Density, Mass Energy Density, and Heat Charge Temperature. Because of this, remanufacturing is ranked first and refurbishing is ranked last. Compared to other options, Mg2FeH6 is superior.

Keywords: MCDM method, MgH_2, Heat charge temperature

1. Introduction

Lithium hydride (LiH), calcium hydride (CaH2), and magnesium hydride are the three chemical hydride systems that have been investigated for thermal energy storage (MgH2). The CaH2 and LiH systems have lately received fewer resources, so in this piece, we concentrate on the MgH2 system of thermochemical storage of energy. The Mg/MgH2 system can function adaptably in the 200–500 °C temperature range and the 1–100 bar hydrogen partial pressure range. Slow hydrogenation/dehydrogenation kinetics and poor resilience of Mg/MgH2 as a TCES material restrict their industrial utility. These issues have been solved using a variety of techniques, including nanostructures, composite inserts, and MgH2-based composites. Numerous organizations have suggested and researched nanostructured materials to overcome the drawback of bulk MgH2 [20]. Examined how grain size affected chemical disorder, internal strain, and grain boundaries during hydride production. The kinetics of hydrogenation were found to be improved by nanostructured materials, which can be attributed to the materials' greater porosity, grain limit, and MgH2 particle reaction surface, along with the shorter inter-hydrogen diffusion distance, are all positive. Utilizing ab initio Hartree-Fock as well as density function theory, the effect of particle size on the thermodynamic stability of Mg/MgH2 was investigated from a micro perspective. Due to the drop in dehydrogenation bond energy with small grain size, their calculation results showed that MgH2 decomposition can be easily carried out at low temperatures. A nano-composite is a term that is frequently used to describe a finished product when a sizable portion of the dopant in comparison to the substrate is used. For instance, when 3.4 wt% release of hydrogen at 3008C is completed in 30 min. rather than 75 minutely. In an Mg ball machined with 35 wt% porous transition-metals alloys, adequate catalytic features are stated. However, the capacity for storing is less than half of magnesium. The reciprocal catalytic properties between various metal hydrides were examined in order to prevent the loss of energy storage brought on by the application of catalysts with inadequate hydrogen storage capacity. It has been noted that combining various hydrides in a ball mill produces amazing effects. The mixing of MgH2 and Mg2NiH4 is a classic example, where the ultimate storage capacity of each remains the same but the more stable hydride is Zaluska et al. The ternary hydride releasing hydrogen at low temperatures creates a larger interface that speeds up the binary hydride decomposition process, which could be one reason for this impact. The sorption characteristics of both phases seem to be maintained, but one of the phases appears to serve as a catalyst for the other, causing MgH2 to release its hydrogen content at 275 C as opposed to 350 C. By offering a methodical, logical, and repeatable approach for various uses and cutting down on the number of erroneous decisions made when choosing materials, MCDM methods are being used more frequently. The choice of appropriate materials typically involves a number of crucial steps, such as ranking and selection, and is dependent on the user's preferences for the intended function [15]. Liao created and put forth a fuzzy multicriteria choice-making method based on trapezoidal fuzzy numbers to help with choosing materials choices in engineering design applications. Using analogies with Cambridge material selection techniques, Farak [5] examined material selection tools such as value engineering (VE), the best solution (TOPSIS), and order selection techniques. Holloway [6] investigated how improper material selection in machine design affected the ecosystem. This research demonstrates how, using Ashby's method, material selection charts can be used to define mechanical design for the best possible environmental impact [7]. In the selection and design of materials, a straightforward multi-objective strategy based on value functions was given by Ashby [8]. Shanian and Sawatoko [9] created a novel method for creating a material selection decision matrix by using criterion sensitivity analysis, Criterion sensitivity analysis, elimination and choice reflecting the reality (ELECTRE) models. Introduced a hybrid multi-criteria decision modeling method that was integrated with a TOPSIS and VIKOR analysis-based analytical network process to choose the best fuel mixture. Additionally, graph theory has recently been used to help solve many actual issues in the field of chemistry. In this area, graph theory offers a visual depiction of chemical compounds and lets researchers concentrate on the physicochemical properties of molecular graphs [19–22]. For heat storage applications, there is a need for an extensive, user-friendly, and target-relevant MCDM technique. This research suggests a general, using a matrix approach and graph theory to fill in the gaps, a user-friendly MATLAB software based on the MCDM method is developed to select thermochemical storage materials. In this study, In order to determine which material would be most effective for medium- to elevated temperatures storage of heat based on actual requirements and user preferences, a target waste heat recuperation unit at Tata Steel's Port Talbot Steelworks was selected. Graph theory is the study of objects (also known as graphs) with a collection of vertices, each couple of which is assigned an event relation denoted by an edge, as part of a formal and logical method. In many different scientific and technological fields, graph theory has offered an especially potent and practical method for modeling and analyzing various systems and the issues that go along with them. Additionally, the matrix method helps to quickly and effectively analyze the obtained graph models [1]. To make decisions and choose materials for high temperature heat storage applications, this paper uses graph theory and a matrix method. Several thermal storage techniques and a variety of materials can be used to accomplish high-temperature thermal storage. Any heat storage system's efficiency and use are influenced by a number of design factors, such as the material, Process, reactor construction, and atmospheric psychrometric conditions [31]. When selecting a material for heat storage, Based on user taste, engineering design requirements, and end users, a number of important factors and parameters ought to be taken into account.

2. Material and Methods

The system needs to be studied to broaden the commercial application of Mg/MgH2 materials. The components of a standard Mg/MgH2 TCES system include a reactor, numerous heat exchangers, Mg/MgH2 storage tanks, and an electric generator. The Mg/MgH2 TCES system's reactor is its most crucial component. Although a fixed bed is infamous for its subpar effective thermal conductivity, it is generally acknowledged as the reactor that is best suited for the charging and discharging stages. Gambini [31] created a bulk factors model for the Mg/MgH2 nuclear power plant in order to increase the fixed bed's heat conductivity. The mass and heat transmission of the Mg/MgH2 TCES system were described using this model. For TES systems, this model can be used to build a furnace's transfer of heat mechanism. The effectiveness of heat transfer for a 2D Mg/MgH2 reactor was later examined by Askri et al. [32] while considering radiation heat transfer into account. The hydrogenation transition has been shown to be highly radiation-sensitive. A mathematical model was created by Shen et al. [33] to examine the impact of metal foam's porosity on the effectiveness of heat transmission in a Mg/MgH2 reactor. According to their study, the presence of metal foam not only encourages the production of exothermic energy but also reduces reaction time by 40%. Particularly when the reaction rate and production capacity peaked, the porosity was 0.96 and the temperature at which the reaction occurred was 620 K. It was discovered that short-term milling with AlH3 can greatly improve MgH2's hydrogen sorption kinetics and start temperature with a molar ratio of 1:1 in the MgH2 + AlH3 mixture. 55 °C is lower compared to pure MgH2. It was hypothesized that the in-situ breakdown of AlH3 brought on by the contact of MgH2 and oxide-free Al* was what caused the improved kinetics and reduced wear temperature. AlH3 also demonstrates superiority over metallic aluminum in terms of its capacity to enhance MgH2's sorption dynamics. AlH3, a superior metal hydride, is brittle and can be quickly ground with MgH2 to allow precise mixing. AlH3 will also break down into the chemically active, oxide-free Al*. The kinetics of the MgH2 and Al reaction are benefited by both of these characteristics. However, little research has been done on the specific decomposition traits and process of MgH2AlH3 composites, and little is known about how these composites behave when storing hydrogen. Sato69 and Iosub70 explored the direct synthesis of magnesium alanate using MgH2 and AlH3 as starting materials, and Iosub71 looked into the stability of AlH3 when MgH2 was added. The MgH2 + AlH3 mixture (1:1) also has a comparatively low reversible hydrogen capacity due to the Al component's inability to adsorb hydrogen under the applied adsorption conditions. Therefore, to achieve comparatively high reversibility in MgAlH alloys, the percentage of AlH3 should be decreased. A goal-based material selection factors diagram is created using the data gathered in the first stage (selection factors and their relative significance), with nodes 1–5 shown in Table 1. The five alternatives' material selection factors' quantitative values (also known as the "factors of interest") are provided in Table 3 and must be reliably normalized. HCT is a non-beneficial component, while HRT, DHEnt, VED, and MED have quantitative values. Table 2 displays the normalized numbers for these five scaling factors. The variation in temperature between the intake and exhaust air is used to compute VED, which is defined as an increase in the thermal conductivity of air. The mass of water lost from the sample and the mass of reaction energy are used to determine MED [4]. In this research, HCT, HRT, and DHEnt all have equal significance with regard to target users. HCT and HRT are not significantly more pertinent than VED, MED, or SPH, and the inter-influence of the requirements is equal. VED, MED, and SPH were more significant than HCT and HRT. This supports DHEnt, VED, MED, HCT, and HRT. Additional relative significance values are offered as an example MCDM matrix for the selection of high-temperature electricity storage materials based on the planned application. Different goals and alternative end-user requirements could lead to specific values that are different from those in this paper. The values in Table 2 can be used to substitute the values for the standardized choice of material variables (R1–R5), which are numerical representations of the heat charge temperatures, heat release temperatures, reaction energy, volume density of energy, and mass-energy density of energy for each material. This section includes an extra illustration to help clarify the strategy and bolster the suggested approach. This practical example focuses on the selection of an appropriate heat storage material for waste heat that is low to medium in temperature (below 200 C). Based primarily on the authors' prior work on salt-enriched desiccant matrices [1,2] for open thermo chemical energy storage, five distinct candidate materials were proposed for this example [1-6]. The goal material selection parameters mentioned in this example are heat charge temperature (HCT), heat release temperature (HRT), reaction enthalpy (DHEnt), and volumetric energy density (VED). The identification of variables of interest that is based on user quantitative or qualitative evaluation of the acceptance value or threshold for low- to medium-temperature thermal storage applications is the fourth step after the first three. Based on the data gathered in the first stage, a map of the target-based material selection factors is created for this example, and its matrix representation is created using the previously stated procedures. Based on [6], Table 2 displays the quantitative values of the material selection factors (factors of worry) for five distinct materials. COPRAS were created initially by Zavatskas and Kaklauskas (presented in 1996). The COPRAS method, which has a higher resolution rate, decides the answer. Clearly state the relative importance of each alternative technique and criterion's values this method's assumption of direct and proportional dependence and utility underlies the significance of the variants that are under investigation. Scale weights and approximations of Soft's alternatives are considered as numerical data in traditional cobras. However, a number of circumstances call for real-world decision-making issues. Smooth input is insufficient for handling. However, accurate information is not always simple to come by. They also contribute to the findings' accuracy.

3. Results and Discussions

Alternative techniques and standards numbers and accurately determine the weights this method is direct and proportional biased and takes usability into account when determining the significance of the versions investigated in the descriptive criteria. Five steps are taken to determine the significance, order of relevance, and extent of use of alternatives: 1. D-matrix for a weighted normal choice. 2. Normalized weighted summarizing the alternative the computation of symbol sums. 3. Benefits of substituting and drawbacks of substituting Describe the options being compared and figure out their Qj values. Application level of substitute AJ 5. Establishing the options' relative importance. To pre-qualify each of the five window replacement variants offered by bidders According to the results of the multi-criteria assessment, the first option is superior when the utilization rate is 100%, and the third version is essentially the second best. Usage percentage is 100 percent. The choice of the contractor will be made in the following stage. Taking into account candidate bids, pre-qualification criteria were met. Following the technical evaluation, the final test of the contractors will be given before the contract is awarded. The technical grade will be correlated with price proposals. Display table 1 and provide assessment criteria.

TABLE 1. Evaluation parameters

Heat Release Temperature	HRT
Reaction Enthalpy	DHEnt
Volumetric Energy Density	VED
Mass Energy Density	MED
Heat Charge Temperature	HCT

The evaluation criteria are displayed in Table 2. (Schemes) Heat Charge Temperature is HCT, Heat Release Temperature is HRT, Reaction Enthalpy is DHEnt, Volumetric Energy Density is VED, Mass Energy Density is MED.

TABLE 2. Given a data set

	HRT [C]	DHEnt [kJ/mol]	VED [kWh/m3]	MED [kWh/kg]	HCT [C]
MgH2	230	75	580	0.80	380
MgH2/Composite	230	60	580	0.80	380
Mg2FeH6	510	77	650	0.54	590
Mg2NiH4	220	62	295	0.25	330
MgO/Mg(OH)2	100	81	380	0.39	150
	B	B	B	B	NB

Table 2 is provided a set of data. The data set's Mg2FeH6 values are elevated. MgH2 values in the data collection are low. The data collection used for the COPRAS method's Material Selection for the MgH2, MgH2/Composite, Mg2FeH6, Mg2NiH4, and MgO/Mg(OH)2 of the HRT, DHEnt, VED, MED, and HCT is shown in Table 1.

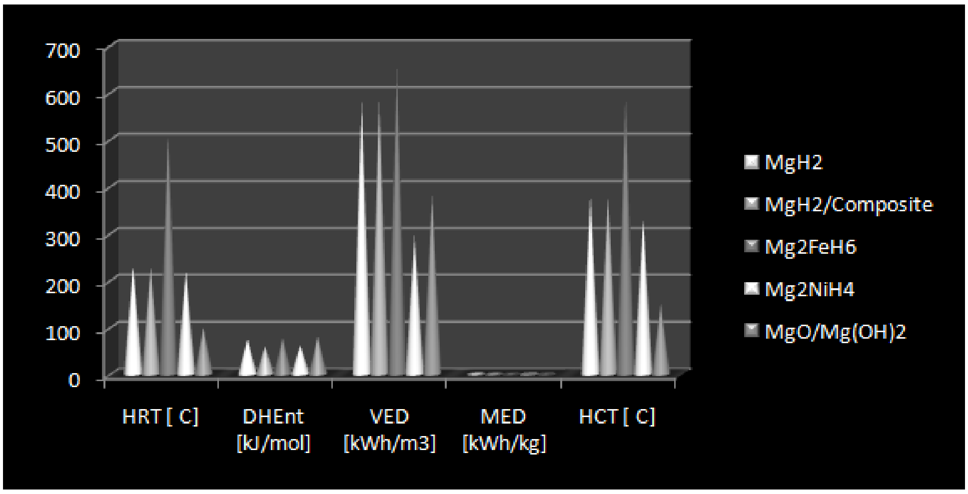

FIGURE 1. Give a data set graph

The data collection for the HRT, DHEnt, VED, MED, and HCT MgH2, MgH2/Composite, Mg2FeH6, Mg2NiH4, and MgO/Mg(OH)2 is shown in Figure 1.

TABLE 4. Normalized data

	HRT [C]	DHEnt [kJ/mol]	VED [kWh/m3]	MED [kWh/kg]	HCT [C]
MgH2	0.1783	0.2113	0.2334	0.2878	0.2077
MgH2/Composite	0.1783	0.1690	0.2334	0.2878	0.2077
Mg2FeH6	0.3953	0.2169	0.2616	0.1942	0.3224
Mg2NiH4	0.1705	0.1746	0.1187	0.0899	0.1803
MgO/Mg(OH)2	0.0775	0.2282	0.1529	0.1403	0.0820

The normalized data from the data set are shown in Table 4; each value is computed by taking the same value from the data set and dividing it by the sum of the corresponding column in the previous tabulation.

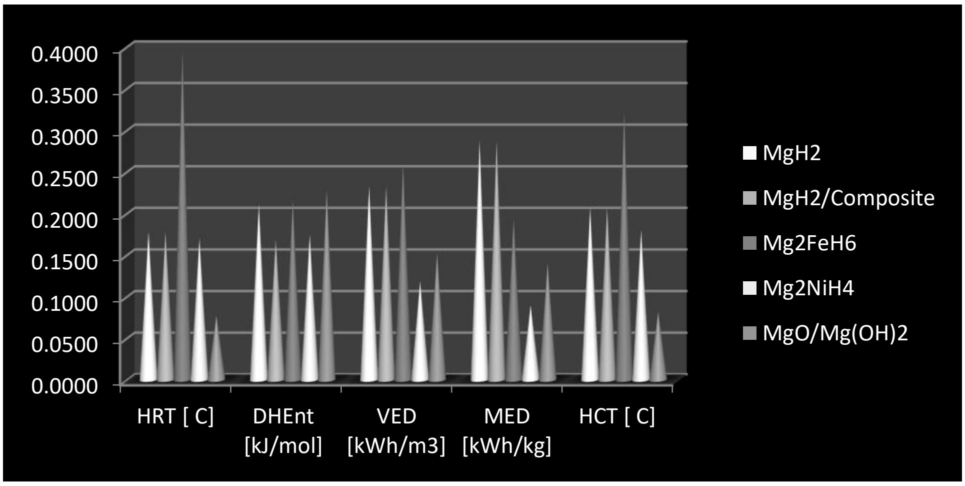

FIGURE 2. Gives the normalized data

TABLE 5. Gives weight matrix

MgH2	0.20	0.20	0.20	0.20	0.20
MgH2/Composite	0.20	0.20	0.20	0.20	0.20
Mg2FeH6	0.20	0.20	0.20	0.20	0.20
Mg2NiH4	0.20	0.20	0.20	0.20	0.20
MgO/Mg(OH)2	0.20	0.20	0.20	0.20	0.20

The weight of the data set, which is identical for each value in the set of data in Table 1, is displayed in Table 5. To obtain the following value, the weight is multiplied by the prior table.

TABLE 6. Weighted normalized result matrix

MgH2	0.04	0.04	0.05	0.06	0.04
MgH2/Composite	0.04	0.03	0.05	0.06	0.04
Mg2FeH6	0.08	0.04	0.05	0.04	0.06
Mg2NiH4	0.03	0.03	0.02	0.02	0.04
MgO/Mg(OH)2	0.02	0.05	0.03	0.03	0.02

The weighted normalization decision matrix, shown in Table 6, is created by multiplying the performance number and weight from Tables 4 and 5.

TABLE 7. Bi and Ci Values

	Bi	**Ci**
MgH2	0.182	0.042
MgH2/Composite	0.174	0.042
Mg2FeH6	0.214	0.064
Mg2NiH4	0.111	0.036
MgO/Mg(OH)2	0.120	0.016

Bi, Ci, and Min(Ci)/Ci are valued in Tables 7 and 8. The sum of the specific strength, specific modulus, and corrosion protection yields the bi. The sum of cost categories is used to compute the Ci.

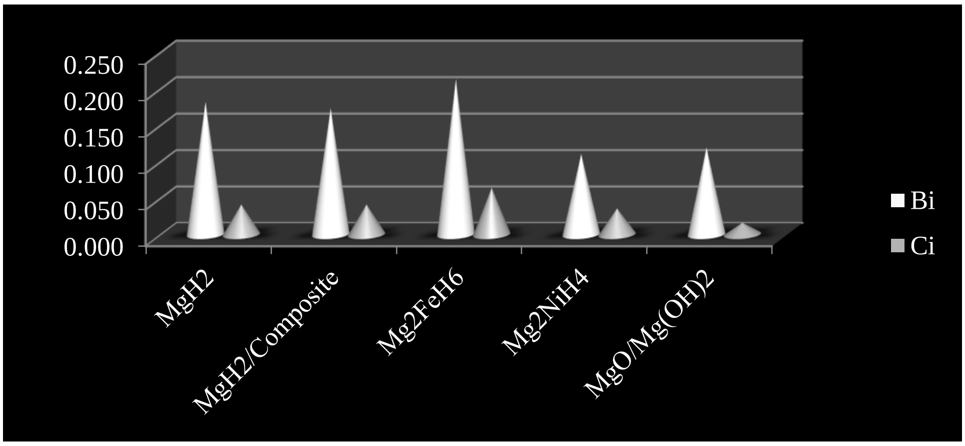

FIGURE 3. Bi, Ci values

TABLE 8. Min(Ci)/Ci, Qi, and Ui

	Min(Ci)/Ci	**Qi**	**Ui**
MgH2	0.3947	0.214	91.3583
MgH2/Composite	0.3947	0.205	87.7464
Mg2FeH6	0.2542	0.234	100.0000
Mg2NiH4	0.4545	0.147	62.8960
MgO/Mg(OH)2	1.0000	0.200	85.4118

Tables 7 and 8 display the values for Qi, Ui, and Min(Ci)/Ci. The Bi and Ci are used to determine Qi, which is then used to calculate the Ui. Qi numbers are used to determine Ui values.

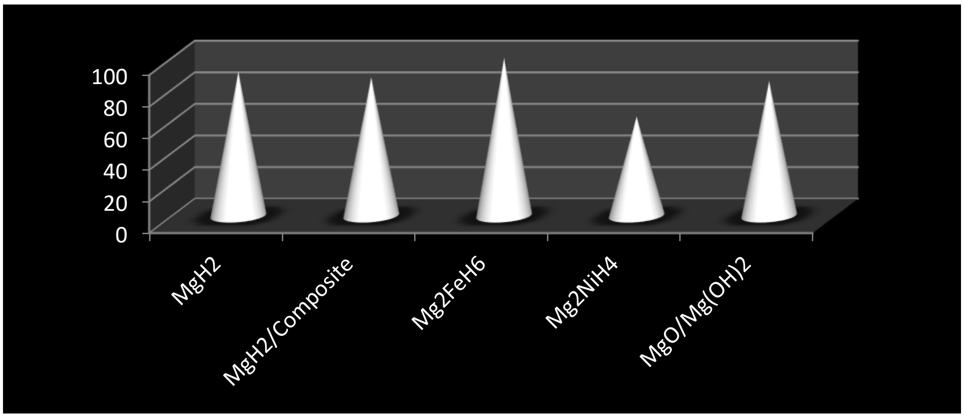

FIGURE 4. Ui values

TABLE 9. Ranking

MgH2	**2**
MgH2/Composite	**3**
Mg2FeH6	**1**
Mg2NiH4	**5**
MgO/Mg(OH)2	**4**

According to Table 8, Mg2FeH6 is on the first position, MgH2 is second, MgH2/Composite is third, MgO/Mg(OH)2 is fourth, and Mg2NiH4 is fifth.

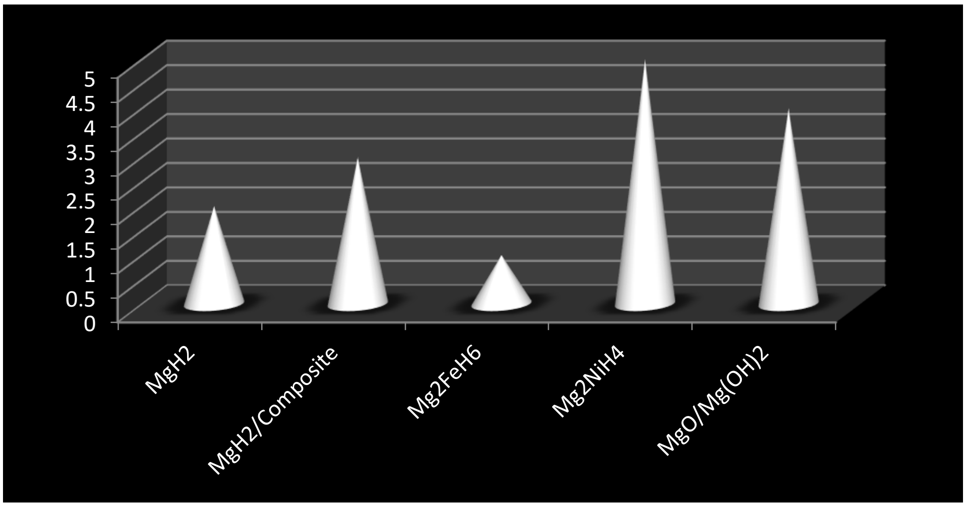

FIGURE 5. Shown in ranking

According to Figure 5, Mg2FeH6 is on the first order, MgH2 is second, MgH2/Composite is third, MgO/Mg(OH)2 is fourth, and Mg2NiH4 is fifth.

4. Conclusion

A suggestion for a multi-criteria decision-making tool is included in this body of work for selecting heat storing devices that use industrial waste heat as a source of heat capture. The method uses graph theory and a matrix strategy to create a goal-based object matching code in a MATLAB program that considers both qualitative and quantitative data sets. This approach enables ranking the relative importance of each element and takes both objective and subjective criteria into account. The real-world test case for the waste heat recovery powers of the MCDM tool is the Port Talbot Steelworks of Tata Steel UK. For the evaluation of two scenarios, the temperature levels of 200 C and 500–600 C are used for waste heat. When temperatures are excessive, five target material selection variables are used altogether, whereas only five are used in the low temperature range. MgH2/Composite and MgH2 are preferred variants in the high temperature region, whereas MgO/Mg(OH)2 is preferred from the (more constrained) lower temperature area. In comparison to recent research in the area and ongoing studies, both sets of material are pertinent. This work's methodology will make it possible to choose candidate materials for thermal storage devices more precisely. Since there are already a lot of candidate systems for thermo chemical storage, this technique can be used to quickly and easily narrow down the options for materials for upcoming research projects.

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