Innovative Methodology and Decision support tool for thermal energy storage material selection

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Abstract–**This work introduces an innovative methodology for the selection of the most adequate materials to be utilized for the commissioning of thermal energy storage units in end-use sectors (namely process industry plants). Such approach is set to be essentially used for heat recovery systems in which the supply of thermal energy (heat source to heat sink) is only possible under specific conditions (considering the limitations associated to standard heat recovery). An innovative decision support tool (designated as TESTool) applying an adapted version of the aforementioned methodology is also presented. The application of the developed methodology is tested through the analysis of a Portuguese can industry plant, in which organic phase change material have been assessed as the most suitable materials to constitute a potential thermal energy storage system.**

Index Terms-- **Thermal energy storage, waste heat recovery, material selection, process industry, decision support tool**

I. Introduction

The principle of progress towards industrial sustainability is based on the reduction of resource consumption and the environmental impacts associated to the waste produced in plants [1]. The most important resources include water, electric energy, fuels and process raw materials. In practice, promotion of industrial sustainability may be performed by improving the overall use of water and energy use, the application of renewable energy resources and the application of waste-to-energy technologies [2].

The concept of circular economy has been emerging to transform waste into potential by-products, promoting reuse, recovery and recycling, in which the life cycles of the production chains are optimised [3]. In the limit, the application of several measures converges on the reuse of resources (either material or energy) within the same industrial site. Waste heat recovery (WHR) systems subsist on the application of energy management principles to plan the installation of WHR technologies to recirculate streams with an associated waste heat potential so to improve energy efficiency and so to promote the circular economy associated to industrial systems [4]. For additional energy supply, thermal energy storage may reveal as a particularly attractive set of technologies, considering its potential to surpass limitations of WHR such as significant distance between the heat source and the heat sink, the lack of identification of existing heat sinks, operation disturbances and overall techno-economic viability associated to the implementation of these technologies [5].

This work approaches the development of an innovative methodology set to be implemented for the process of selection of thermal energy storage (TES) materials in the context of specific cases of end-use sectors (with focus on industrial plants). It also presents the development of a computational decision support tool, built according to the principles defined in the aforementioned methodology. A case-study set within a Portuguese can production plant is approached for the purpose of validating the developed methodology.

II. Methodological Framework

The selection of TES materials in the context of energy-using processes depends on a number of factors, namely:

- Operational factors;
- Physical-chemical properties of materials;
- Economic factors;
- Market availability and technology maturity;
- Safety and regulatory factors.

The most accurate methodology for TES selection must consider the identified general criteria (with criterium each being associated to its relative importance) with the objective to classify the set-to-be-analysed materials. Owing to the wide range of available TES technologies and the diversity of energy-using processes and specific requirements, the application of such methodology shall be significantly complex, which may limit the adoption of TES systems under development in the market.

The methodological framework developed in the scope of this work is divided into two execution mechanisms:

1. **The most general methodology** considering the afore identified criteria in a general manner, subsisting in the comparison of the aspects associated to specific

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operational conditions of a site (e.g. an industrial plant) and aspectual advantages and disadvantages of TES categories. The main objective of this work is to prove the validity of this tool in terms of the selection of TES materials for specific case-studies;

2. **The more specific TESTool** decision support tool, which considers an assessment of benefits based on the attribution of numerical quantities to a set of indicators related to each one of the afore identified criteria.

III. TESTool – TES Selection Decision Support

To increase the chances of success in implementing this type of system, it is essential that decision-makers have access to a tool that helps them assess and interpret the potential of TES materials. In this prospect, a computational decision support tool is being developed, with the aim to assess the most suitable TES material selection using a criteria-based matrix. This program is set to generate radar graph-based results that will allow an initial approach for material selection. The aim is for this tool to be suitable for both customers and all stakeholders in the value chain.

The considered material selection criteria subsist on the expansion of the factors identified in section II.

- For some properties, such as chemical stability or moldability, it is quite difficult to assign values for the categorization of the selection matrix. Thus, the value considered is simply ‘na’ (i.e. not applicable), and therefore, to facilitate data processing, it was determined that this value would be 5;
- Other properties, such as the vapour pressure of TES-sensitive materials or their availability, are particularly difficult to designate quantitatively, so a qualitative scale (*Low, Medium Low, Medium, Medium High, High*) was chosen. These values were chosen by consulting reference documents/bibliography. In the case of solid TES-sensitive materials, such as aluminium or granite, it is not possible to associate a vapour pressure, since the temperatures at which the change of state or degradation occurs are very high and, therefore, these materials are considered to always remain in the solid phase;
- The values of thermochemical TES materials were analysed with some caution due to the relatively lack of information in relation to the other categories (only the temperature and reaction enthalpies being known in detail), as well as due to the low TRL (between 3 and 5) of these types of materials, so most of the properties were analysed in a qualitative way;
- Some TES sensitive materials are considered in a generic manner, as a group of materials rather than a specific material (e.g. thermal oil or molten salts), so the value assigned corresponds to an average of the values found in the literature.

In Figure 1, it is represented a general conformation for the radar chart obtained as a result of running a simulation in TESTool. In Table I, each one of the considered criteria-based parameters are characterized in detail. The aspects related to the definition of the criteria-based matrix, presentation of numerical and qualitative assessments and radar graph-based results from TESTool are presented in the Appendices section of this work.

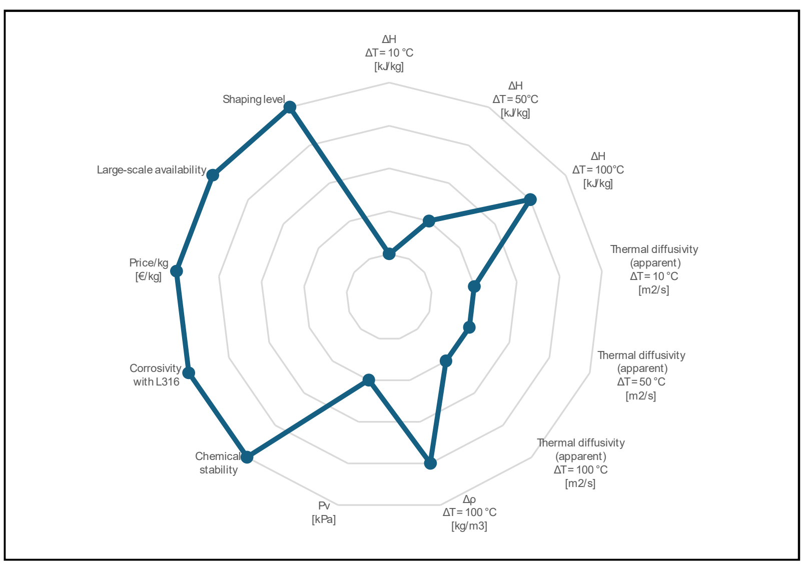

FIGURE 1. GENERAL CONFORMATION OF THE RADAR CHART OBTAINED AS A FINAL RESULT ON TESTOOL

TABLE I. SELECTION CRITERIA FOR THE DECISION SUPPORT TOOL

Selection criteria		Units
Variation of specific enthalpy (ΔH)	ΔT = 10 ºC	kJ/kg kJ/m³
	ΔT = 50 ºC	
	ΔT = 100 ºC	
Apparent thermal diffusivity (α)	ΔT = 10 ºC	m² /s

	ΔT = 50 ºC	
	ΔT = 100 ºC	
Apparent density (ρ)	ΔT = 100 ºC	kg/m^3
Vapour pressure (P_v)		kPa
Chemical stability		Dimensionless (Number of cycles)
Corrosivity (with AISI 316L stainless steel)		g/year mm/year
Specific cost		€/kg
Availability		Dimensionless
Ability to shape		Dimensionless

IV. INTEGRATION OF AN INDUSTRIAL CASE-STUDY

In the scope of the present work, a case-study set within a can production plant installed in Portugal is set to be analysed for the purpose of validating the developed methodological framework. For the fulfilment of such purpose, a primary analysis subsisting on the characterization of the existing heat sources and potential heat sinks within the mentioned plant have been proceeded. Such analysis resulted in the assessment of the following aspects:

- The considered heat source would be an incinerator, more properly the outlet exhaust gases streams;
- The considered heat sink would be an adsorption chiller, more properly the inlet water stream.

In Figure 2, a flowsheet-based representation of the integration between the heat source, the heat sink and the TES unit is performed.

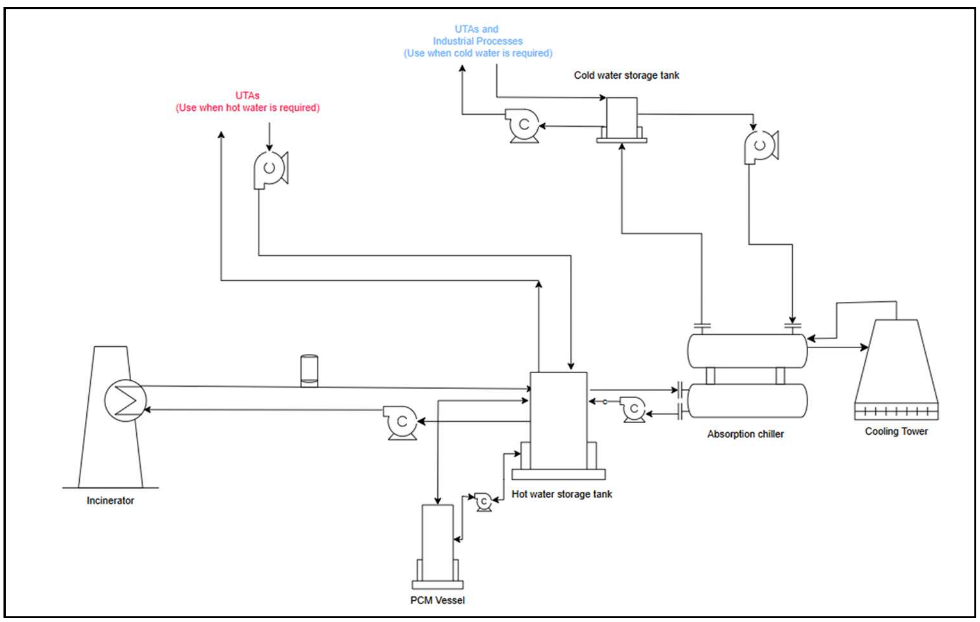

FIGURE 2. FLOWSHEET ENCOMPASSING FOR THE TES SYSTEM

For the purpose of the execution of the foremost objective of this work associated to TES material selection for a specific case-study, the **execution mechanism 1** (most general methdology) will be used. Although the overall potential associated to TESTool has been demonstrated in section III, this tool still has to suffer significant improvements in terms of automatism, user-friendliness and the inclusion of more detailed information.

The preliminary selection of heat storage materials and technologies (TES) depends on a primary analysis of each of the categories of materials/technologies already explored [6]–[8] in relation to the operating conditions of the approached can production plant, namely the heat source and sink previously identified. Table II presents the aspects related to the suitability of each category of heat storage material with the operating conditions associated with the plant. Table III presents the aspects related to the suitability of several categories of latent thermal energy storage (LTES). It should be noted that the aforementioned tables serve to assist in the preliminary selection of the TES with the greatest potential by identifying the advantages and disadvantages associated with each of the categories, and at a later stage by verifying these advantages and disadvantages in relation to the case study described, namely through the following identification by colours:

- Highlighted (white letters): Positive point, in which an **advantage is verified** or a **disadvantage is not verified**;
- Non-highlighted: Neutral point, where an **advantage or disadvantage has no associated impact**;
- Highlighted (black letters): Negative point, in which an **advantage is not verified** or a **disadvantage is verified**.

TABLE II. SUITABILITY OF EACH MAIN CATEGORY OF TES MATERIAL TO THE CASE-STUDY CONDITIONS

Heat Source		**Flow rate: 26000 m³/h, Temperature: 170.0 °C**	**Heat source after TES**	**Temperature (max.): 100.0 °C (at 1 bar)**
Cat.		**Sensitive**	**Latent**	**Thermochemical**
Advantages	General	1. High energy storage capacity 2. Low cost of storage materials 3. Inability of solid media to freeze and be able to achieve high temperatures 4. Relatively simple application (for the available materials)	1. Suitable for isothermal or low-temperature applications 2. Potential to provide a high energy density, when combined with sensitive TES 3. Average energy density 4. Possibility for transportation in a short distance	1. High energy density 2. Low heat losses 3. Potential for long-term energy storage 4. Compact storage system 5. Possibility for transportation in a short distance
	Case-study	1. To carry out the project in question, it is necessary that the selected TES materials have the greatest storage capacity possible 2. Material costs depend (subjectively) on the selection of storage material by industrial representatives, not depending on exactly one objective analysis 3. The inability of sensitive TES solid materials to freeze is an added value, since associated problems (such as corrosion) do not occur, and the achievement of the highest possible temperatures are reached is also a desirable characteristic 4. The implementation of TES systems must be performed in a relatively simple manner	1. The heat source that will be used directly in the TES systems presents a relatively low temperature relatively 2. The TES system to be commissioned will (in principle) consider a single TES unit 3. An average energy density is acceptable for the approached TES system 4. The possibility of transporting the storage system in a short distance is propitious to the approached system, in which the distance between the heat source and heat sink is relatively low	1. The selected TES material shall desirably be associated to the highest possible energy density 2. Low heat losses are highly desirable 3. The system to be commissioned not necessarily requires long-term storage, since it essentially serves for the establishment the enthalpy transfer of a heat source and a heat sink within a same plant (with the source and the sink not necessarily being in operation at the same time) 4. A higher compression of the TES system is desirable (to avoid the highest level of occupation of space of this system) 5. The possibility for transportation in a short distance is propitious to the approached system, in which the distance between the heat source and the heat sink is relatively low
Disadvantages	General	1. Insulation requirement (to reduce heat losses) 2. Requirement for larger volumes (owing to relatively lower energy densities) 3. Freezing of molten salts at temperatures close to 200 ºC 4. Considerable heat losses (depending on the type of insulation)	1. Potential for corrosion 2. Need for cascade systems for higher temperatures 3. Low thermal conductivity 4. Considerable heat losses (depending on the type of insulation)	1. High complexity 2. High investment costs 3. Potential requirement for gaseous products
	Case-study	1. The TES units to be commissioned must be sized *a priori* for heat losses to be the lowest for the lowest thermal insulation installation requirements 2. The TES units to be commissioned must have the smallest possible volume, to occupy the least possible space in the plant 3. The freezing problem associated with molten salts must be avoided 4. Heat losses should be avoided as much as possible	1. The occurrence of corrosion shall be avoided 2. The need for cascade systems shall be avoided 3. Thermal conductivity influences the enthalpy transfer times (from the heat source to the TES material and from the TES material to the heat discharge) 4. Heat losses shall be avoided	1. The systems to be commissioned shall not be associated to a complex structure 2. Material costs depend (subjectively) on the selection of storage material by industrial representatives, and do not depend exactly on an objective analysis 3. The use of gaseous products shall be avoided as much as possible to avoid associated problems such as corrosion.

TABLE III. SUITABILITY OF EACH MAIN CATEGORY OF TES MATERIAL TO THE CASE-STUDY CONDITIONS

Cat.		**Organic**	**Inorganic**	**Euthetic**
Advantages	General	1. Relatively low undercooling requirements 2. Chemical and thermal stability 3. High fusion enthalpy and low corrosion 4. Availability in wide temperature ranges 5. Good compatibility with other materials	1. High thermal conductivity 2. High phase change enthalpy 3. Low volume and cost	1. High volumetric heat storage density 2. Low melting temperature range
	Case-study	1. The undercooling problem shall be avoided as much as possible 2. The TES material to be selected must be associated with the highest possible chemical and thermal stability 3. A high enthalpy of fusion favours the purpose of heat storage, and the corrosion problem shall be as low as possible 4. The associated operating temperature ranges shall be as wide as possible 5. The TES material to be selected shall have the greatest possible compatibility with other materials	1. Thermal conductivity influences the enthalpy transfer time (from the heat source to the TES material and from the TES material to the heat discharge) 2. A high phase change enthalpy favours the purpose of heat storage 3. The storage volume should be as low as possible, although the the material costs depend subjectively on the selection of storage material by the industrial representatives, and do not depend exactly on an objective analysis	1. The energy density should be as high as possible to ensure enthalpy storage in the smallest amount of TES material possible. 2. The melting temperature range is not an aspect that influences the selection of TES material for the case in question.
Dis adv	Ge ner	1. Low thermal conductivity	1. Potential undercooling and corrosion	1. Low thermal conductivity

	2. Relatively high variation of volume 3. Flammability	2. Potential phase separation 3. Lack of thermal stability	2. Potential for corrosion at high temperatures
Case-study	1. Thermal conductivity influences the enthalpy transfer time (from the heat source to the TES material and from the TES material to the heat discharge) 2. The volume variation associated with the TES material shall be accounted for the sizing procedure (which itself does not constitute a problem) 3. The problem of flammability shall be avoided as much as possible	1. Undercooling and corrosion problems shall be avoided as much as possible 2. Phase separation shall be avoided as much as possible 3. Thermal stability shall be ensured as much as possible	1. Thermal conductivity influences the enthalpy transfer time (from the heat source to the TES material and from the TES material to the heat discharge) 2. The corrosion problem shall be avoided as much as possible

Based on a global analysis of the content presented in Table II and III:

- Latent heat storage (using phase change materials (PCM)) is clearly the most viable option for the approached case (highest number of verified advantages and lowest number of verified disadvantages);
- Within this category, it is necessary to assess whether the phase change material to be selected fits into the various categories of this type of material (in a similar way to what was done for each of the three primary categories of TES. Considering a global analysis of the content presented in Table III, TES using organic phase change materials is clearly the most viable option for the case study in question.

V. Conclusions

This work approaches the development of an innovative methodology for the selection of the most suitable materials to constitute thermal energy storage (TES) systems existing or set-to-be-installed in process industry plants. A computational decision support tool has been also developed.

In relation to the two assets developed for this work, it is possible to perform the following affirmations:

- The overall developed methodology is adequate for the purpose of the selection of the most suitable TES materials, considering not only the technical viability associated to Engineering projects but also the sustainability promotion potential (which is requirement supposed to be achieved, owing to the categorization of the installation of this type of systems as energy efficiency improvement projects);
- The approached case-study (can production plant) proved the successfulness of the implementation of the overall methodology in practice (having been estimated a precise selection of an organic PCM);
- The developed tool has been proved to be suitable in terms of the consideration of a high number of selection criteria, and it is effectively faithful to the also developed methodological framework;
- The developed tool must be furtherly developed in the prospect to promote its automatism, user-friendless and the consideration of a higher number of TES materials;
- Nonetheless, such requirement of further development of TESTool effectively does not affect the main objective of the work in respect to the validation of the approached methodology through its application in an industrial case-study.

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APPENDICES

The innovative TESTool has been developed to constitute a simulation tool oriented to the execution of the task related to the selection of thermal energy storage (TES) materials which are more adequate for a determinate heat recovery system project.

The version of the tool at the date of the development of this work only contains text on the Portuguese. Further versions of the tool (namely those set to serve to public releases) are set to contain the corresponding text on English.

The tool is constituted by two main modules:

- The *Database* module, in which the 1 – 5 numerical values associated to each parameter of interest are associated to each TES material. The default values have been defined by the developers based on several techno-scientific considerations, although these may be dynamically changed by the end-users, owing to the subjectivity and variability associated to some of the indicators (for instance, the availability associated to the supply of TES materials highly depends on geographical and seasonal aspects, which may be more adequately defined according to the knowledge of the specific case detained by the end-users);
- The *Simulation* module, in which the parameters of a simulation may be defined, and from which it may be run.

In the sequence of Figures A1 – A3, the general apparatus of the tool in terms of the definition of parameters, access to the modules of the tool and simulation results are presented.

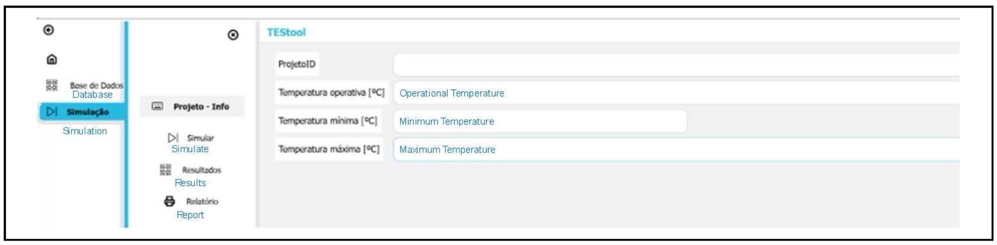

FIGURE A1. FUNDAMENTAL PARAMETERS FOR THE SIMULATION OF THERMAL ENERGY STORAGE MATERIAL SELECTION (TEXT IN PORTUGUESE TRANSLATED TO ENGLISH IN A LIGHTER COLOUR)

Material	Temperature range [°C]	Melting temperature [°C]	Storage type	ΔH ΔT = 10 °C [kJ/kg]	ΔH ΔT = 50°C [kJ/kg]	ΔH ΔT = 100°C [kJ/kg]
Mineral oil	200 - 300		Sensible Liquid	1	2	3
Syntethic oil	250 - 350		Sensible Liquid	1	1	2
Nitrite salt	250 - 450		Sensible Liquid	1	1	2
Nitrate salts	265 - 565		Sensible Liquid	1	1	2
Liquid sodium	270 - 530		Sensible Liquid	1	1	2
Water	0 - 100		Sensible Liquid	1	2	4

FIGURE A2. EXAMPLE OF THE ORGANIZATION OF SOME PROPERTIES AND MATERIALS IN THE THERMAL ENERGY STORAGE MATERIALS DATABASE TESTOOL.

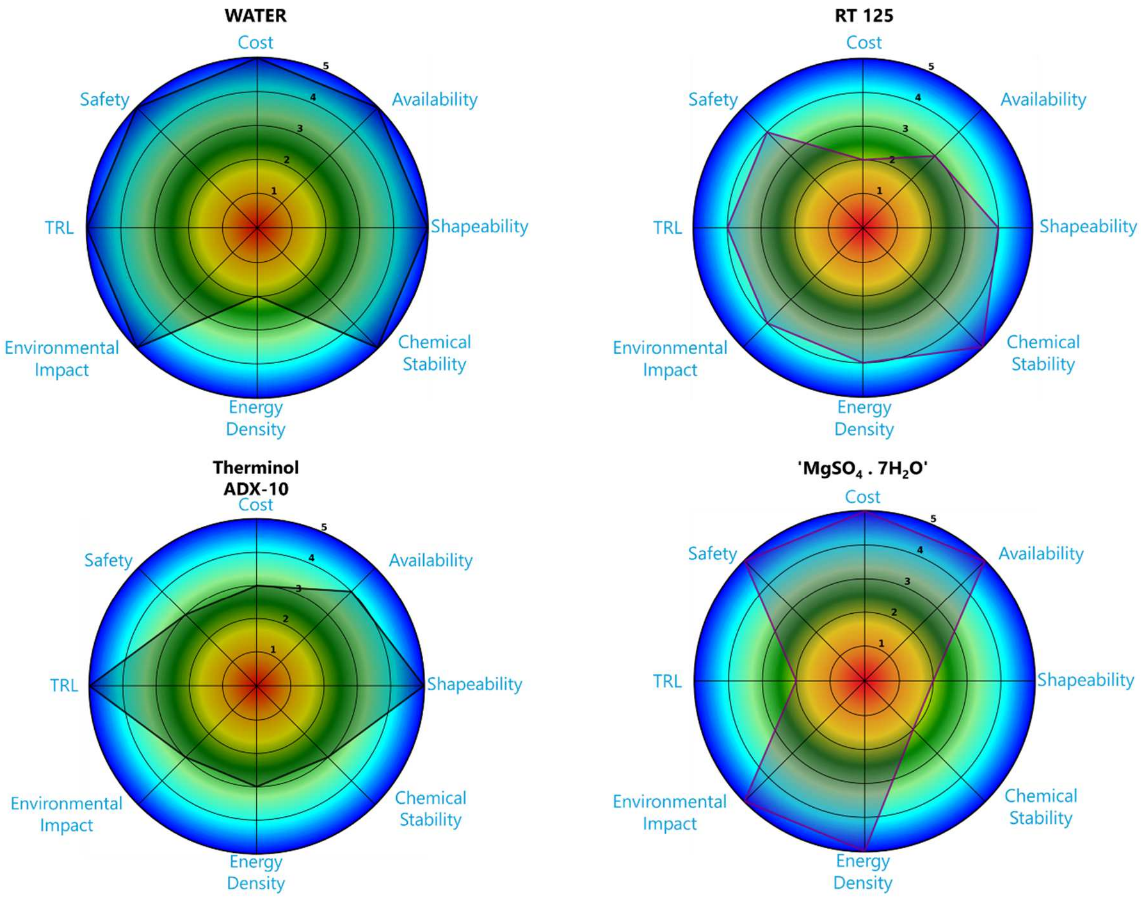

FIGURE A3. SIMULATION RESULTS OBTAINED IN TESTOOL.