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Life Cycle Assessment of thermal energy storage materials and components

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Abstract

The main objectives of research on innovative materials (phase change materials, PCM, or thermochemical materials, TCM) for thermal storage are the development of low-loss and compact storage systems with high capacity (sensible water storages being the benchmark). If the storage is to be implemented in an application with the aim to increase its energy efficiency, beside the technical/thermal properties and cost factors, also the environmental impact of the storage production and operation need to be considered during development. Yet up to now, a holistic development approach that considers the primary energy used for the manufacturing, operation and disposal in relationship to the potential energy savings does not exist for innovative storage concepts. Therefore, we are presenting data on the environmental impact of PCM and TCM on material and component level developed within the German project "Speicher LCA" (engl. "Storage Life Cycle Assessment"). The evaluation shows that PCM can be environmentally beneficial compared to water, if they are used in an application with a small useful temperature difference (e.g. cooling). Storing solar thermal heat with solid sorption materials in a closed system does not seem environmentally beneficial. Additional scenarios assuming the possible reuse of undegraded material, configurations with open sorption storage and/or other material classes (such as salt hydrates and liquid sorption) will be studied in the future

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1. Introduction

When innovative storages (based on phase change or thermochemical materials, PCM/TCM respectively) are investigated the objective to increase the energy efficiency in the housing sector (either by facilitating the use of renewable energy or by load shifting), it is essential to not only evaluate their thermodynamic properties and costs. For a comprehensive evaluation, also their environmental impact during their entire life cycle (including production, use phase, dismantling and disposal) must be considered. In this context the standardized methodology of Life Cycle Assessment (LCA) is applied to PCM and TCM in this paper. After a general introduction on the topic, the ecological impact is first studied on material level. In a second step, also the component level – including all periphery required to build a storage component from the material – is analyzed for PCM. The final step, the incorporation of the storage component in a supply system, is discussed quantitatively and will be available for evaluation in a software tool in the near future.

Nomenclature

A	Adsorption potential [J/g]
$c_{p,sorb}$	specific sensible heat capacity of sorbens [J/g/K]
c_{stor}	specific storage capacity (sensible and sorptive) [J/g]
EER	Energy Efficiency Ratio
h_{evap}	Evaporation enthalpy [J/g]
N_{cycle}	Cycle Number
PE	Primary Energy [J]
T	Temperature [K]
X	Uptake [g/g]

2. Methodology and results

2.1. General descript of LCA methodology

The method of LCA has been developed in order to better understand and address potential environmental impacts of products as well as services. In course of an LCA, the potential environmental impacts (emissions and consumption of resources) of a product along its production chain, use, end of life, recycling and final disposal are analyzed. Thus, LCA allows identifying possibilities to enhance the environmental performance of a product without creating a shift of burdens. Moreover, LCA provides guidelines for decision-makers in industry, politics and non-government organizations. To conduct an LCA, a comprehensive model of the product has to be created based on the material and energy related inputs and outputs of each process of the life cycle of a product as depicted in Figure 1. As the required amount of data is quite extensive, the data collected primarily is complemented by generic information and

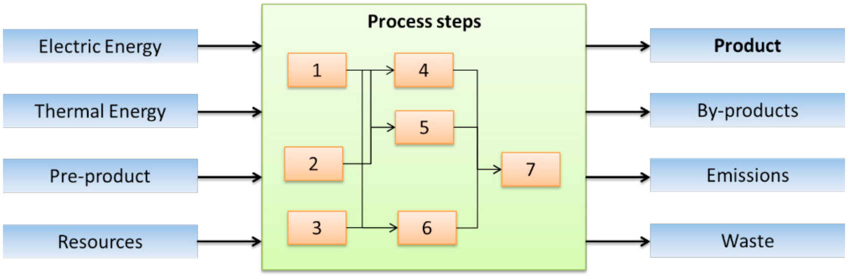

Fig. 1: Required information for the LCA of an exemplary process

background databases, representing technological and market average processes. When put together, the materials entering (resources) and leaving (emissions) the system are characterized in impact assessment using scientifically sound methods to assign the emissions and resources to environmental Areas of Protections that they are impacting.

The LCA method is based on existing ISO standards 14040 [1] and 14044 [2]. These have been complemented with the European standards EN 15978 [3] and EN 15804 [4] for building products in order to ensure the comparability of LCAs. Goal of the European standard is to give a clear guidance for building assessments and environmental product declaration (EPD). Further guidance in the construction sector is provided by the EeBGuide, which supports practitioners in conducting LCA studies and applying the required standards and guidelines (www.eebguide.eu).

In the case of building related assessments, the standard EN 15978 suggests the application of a number of impact categories to comprehensively address the relevant areas of protection. They also include indicators that depict additional environmental effects on resources and waste. Among others Global Warming Potential (GWP), the ozone depletion potential, acidification potential and eutrophication potential are suggested. In case of environmental indicators, primary energy demand (PENRT, comprising energetic and material use), fresh water consumption and the amount of different types of wastes and materials for recycling are recommended. In this paper we base the evaluation on one impact category (GWP) and one environmental indicator (PENRT) since these are the factors typically taken into account when discussing the building stock in context of climate change. While the categories addressing land use, water stress, ecological and human toxicity are relevant for a comprehensive evaluation, beyond doubt, they are not recommended in the standards and consequently not considered here due to their complexity and challenges in application and interpretation, which makes it very difficult to evaluate the results in a generic way, not linked to specific production facilities and locations [5].

The LCA results presented in the following were modelled with the software suite GaBi (http://www.gabi-software.com).

2.2. Environmental evaluation of Phase Change materials and storages

Two groups of PCM, which are suitable for heating and cooling in buildings, are considered in this study: paraffins and salt hydrates.

Paraffin production is mostly based on fossil oil, but materials derived from renewable resources have also been developed [6]. Currently, only fossil-based material have been analyzed due to the lack of information on the latter. Yet in the future, both production paths will be considered for the LCA. The production process is very similar for all the fossil based materials, independently of the resulting length of the carbon chain which determines the melting point. Thus, the specific environmental impact is considered identical for the single materials. The materials relevant for application in buildings (melting point between 0°C and 60°C) have melting enthalpies in the range from 150 to 250 kJ/kg [7], so these two extremes are considered for the subsequent evaluation (described by the suffixes LE and RE for low and high enthalpy respectively).

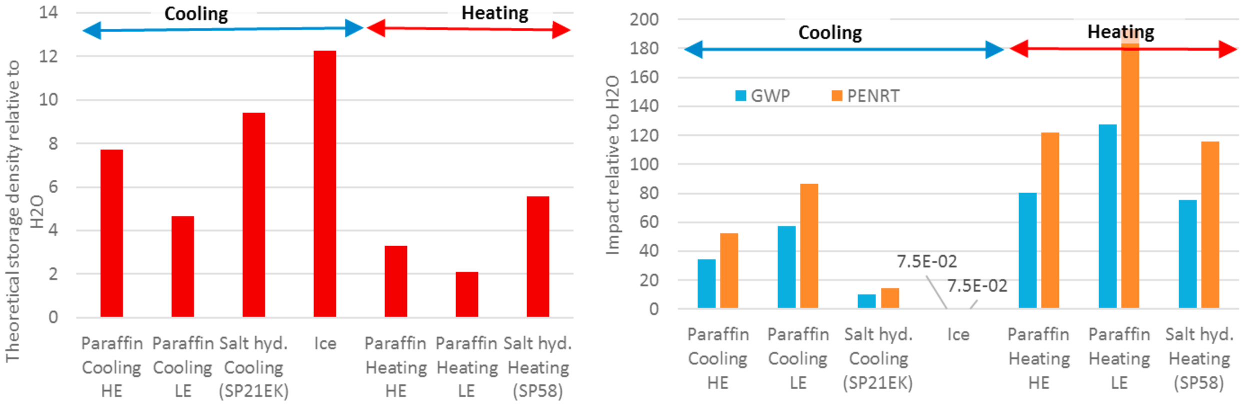

Fig. 2: Left: Volume-related storage density of the considered PCMs relative to water; Right: Impact of PCM production and disposal in the two considered categories; 6K and 15K useful temperature difference considered for cooling and heating application respectively; LE: low melting enthalpy paraffin (150kJ/kg). HE: high melting enthalpy paraffin (250kJ/kg)

The production process of salt hydrates includes the extraction, the purification and the treatment of the primary materials. The materials relevant for cooling in buildings (melting point between 0°C and 25°C) have melting enthalpies around 180 kJ/kg, SP21ET by Rubitherm GmbH is selected as representative for this group. Being the most prominent representative in this class, SP58 (containing Sodium acetate as PCM) with a melting temperature of ~57°C and melting enthalpy of 250kJ/kg is analyzed for heating purpose. Ice with its outstanding melting enthalpy of 333.5 kJ/kg is also included in this study as PCM.

In the left graph of figure 1 the storage density of the considered materials relative to that of water is depicted, assuming a useful temperature range of 6K for cooling and 15K for heating. Values range from ~5 to ~12 for cooling, where the smaller temperature range favors PCM, and 2 to 6 for heating.

In the right graph, the impact of the PCM relative to that of water with the equivalent storage capacity is presented. The global warming potential (GWP) of the paraffins is between 40 to 70 times higher than that of water when used for cooling (with 6K temperature range). When applied for heating purposes these numbers increase to 80 and 130, due to the larger temperature spread which favors water as sensible storage material. The salt hydrate used in SP21EK has the lowest GWP impact, still 12 times more than water. Sodium Acetate shows from a higher environmental footprint with a GWP ~80 times above that of water. The PE trend generally corresponds to that of GWP, absolute values are somewhat higher.

$$N_{cycle} = \frac{PE_{Production} + PE_{EoL}}{\frac{PE_{electricity}}{EER}} \tag{1}$$

Not surprisingly, the intermediate conclusion is, that all the considered PCM have a higher environmental footprint than water. So, from an environmental point of view and ignoring other boundary conditions, on material level water should be the first choice as storage material. Nevertheless since other reasons, such as aspired storage density, may suggest PCM as promising, a further analysis is made: assuming that a) the energy released by the PCM is renewable and b) replaces energy delivered elsewise by a reference system (a chiller with an EER of 3 in case of cooling, a gas boiler with a gross efficiency of 0.9 in case of heating) and c) ignoring the auxiliary system required to charge the PCM, the required number of cycles needed for the PCM to amortize in terms of embedded energy is determined. Equation 1 describes the calculation for PE and cooling; to determine the cycle number for amortization based on GWP, the PE values are substituted by the corresponding GWP values. In case of heating, the factor for electricity and the EER of the chiller are replaced by the value for gas and the boiler efficiency respectively.

The result graph (figure 3) shows that paraffins amortize after ~150 to 260 cycles and 100 to 160 cycles when replacing energy from the assumed reference systems with renewable cold or heat, respectively. Assuming a useful lifetime of 20 years this means a minimum of 7.5 to 13 and 5 to 8 cycles per year, respectively. As before, the salt hydrate used in SP21EK shows the best values – it requires around 40 cycles (or 2 cycles per year) for amortization. Renewable heat extracted from sodium acetate would amortize after 100 cycles (5 per year) against a reference gas boiler.

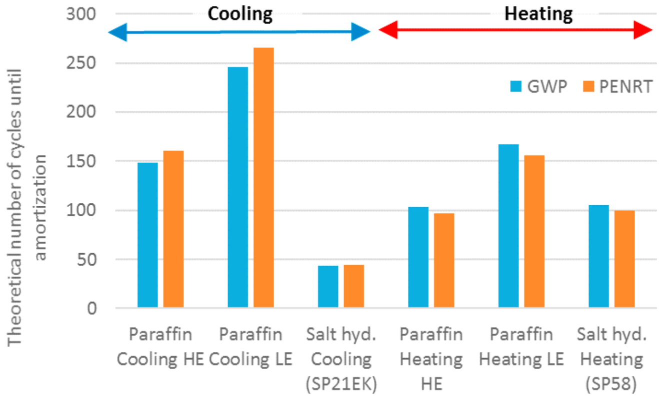

Fig. 3: Number of cycles required for amortization against a reference system

As a PCM requires at least some containment and possibly some auxiliary components it is essential to include those in the environmental evaluation. Therefore, three different storage configurations based on a cylinder with 1m³ volume and 0.8 m diameter are evaluated in this part (configuration see Table 1). The heat transfer medium is water. External auxiliary components, such as three-way-valves to invert the flow direct for charging and discharging PCM storages, and thermal losses are not included in the evaluation.

Table 1. Keydata of the compared storage configurations.

Type of storage	**Volume share of components**	**HX description**
Aluminum based macrocapsules	20% water (in case of ice water+glycol), 13% HDPE capsules, 67% PCM	Configuration derived from FlatICE capsule by PCM Products Ltd. [8]
Immersed heat exchanger based on capillary mats	1% capillary tube heat exchanger, 1% water (+glycol), 98% PCM	2385 m of capillary tube per m³ of storage volume (corresponds to 26.2 m²/m³ specific heat transfer area) derived from [9]
Immersed tube fin heat exchanger (Cu/Al)	1.8% tube fin heat exchanger, 1.5% water (+glycol), 96.7% PCM	157.4 m²/m³ specific heat transfer area, 0.15mm fin thickness, 12mm copper tubing

In a first step, the decrease in storage density compared to water is determined. As the materials change their volume during phase change, the maximum density (solid for water/ice, liquid for all other) is considered therefore. Also, the heat exchangers and the heat transfer fluid further reduce the useful space for PCM. As figure 4 shows, the decrease is similar for the considered heat exchanger variations. For the macrocapsules it is more pronounced because of the assumed volumetric share of 20% water and 13% capsules, which leads to a PCM share of only 67%.

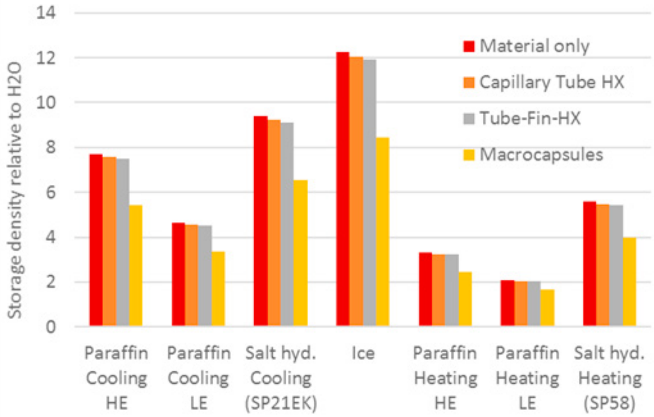

Fig. 4: Storage density relative to water for the three studied storage configurations

In figure 5 the environmental impact in terms of GWP and PENRT per storage capacity in relation to the respective values of a sensible water storage with the same geometry are depicted. It strikes that all but one material in combination with the immersed heat exchangers have a lower environmental impact under the conditions assumed for cooling operations than water. Only the low enthalpy paraffin is unfavorable compared to the reference. The relatively low storage capacity of the sensible water cylinder due to the small useable temperature difference in cooling operation and the high GWP caused by the production of the cylinder and (to a lower extend) the insulation, cause a rather high specific GWP per storage capacity. In other words it could be said that the high impact of the cyclinder and insulation is utilized inefficiently with water as storage medium, if the available temperature difference is small.

The larger useable temperature difference assumed for the heating application changes the picture: here water is the more environmentally friendly storage option, although the difference to the PCM variants is in the single-digit range. This is a substantial change in comparison to the result obtained on the material level (right graph in figure 2), where the values were a factor ~40 higher. Storages based on capillary tube heat exchangers in general have the lowest impact, followed by tube-fin heat exchangers and macrocapsules. The differences are small even in case of the macrocapsules, despite the lower storage density. Here the lower impact due to less PCM compensates the lower density.

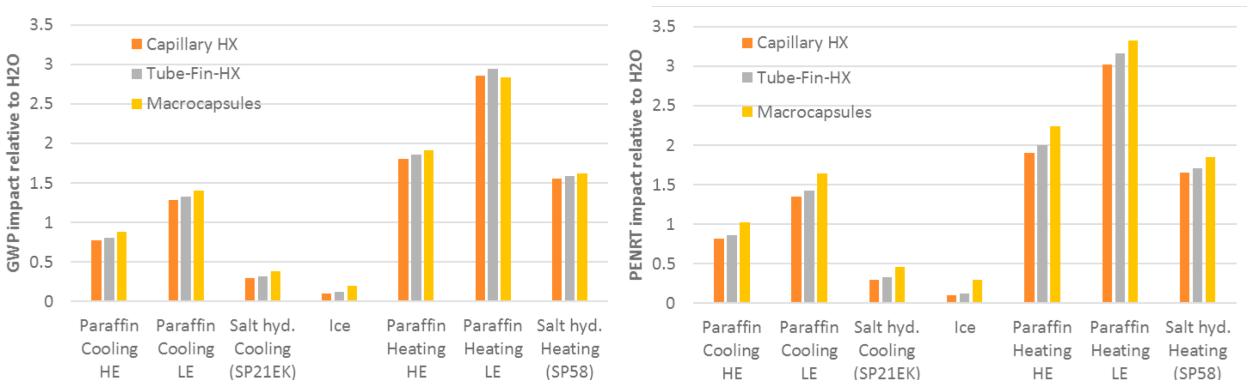

Fig. 5: GWP in relation to storage capacity, separated by storage parts for different configurations; the dashed lines mark the water storage for cooling (blue) and heating (red) as "benchmark"; *25% ethylene-glycol-water mixture in case of the ice storage

As the previous graphs generally show similar trends for GWP and PENRT, in the following results concentrate on the first. For a better understanding of the results, figure 6 illustrates the GWP of the single components separately in relation to the resulting storage capacity for each of the studied configurations. The containment (storage cylinder: 75%) and insulation: 23%) account almost for the entire environmental footprint of the water and ice storages (98%). With the comparably low capacities of the sensible water storages (especially in case of cooling with only 6K) this footprint is "used" rather inefficiently. On the other hand, those PCM configurations with high storage density compared to water "use" this footprint (which is constant in absolute values) more efficiently and can thus lead to a lower specific overall footprint, despite the high impact of the PCM.

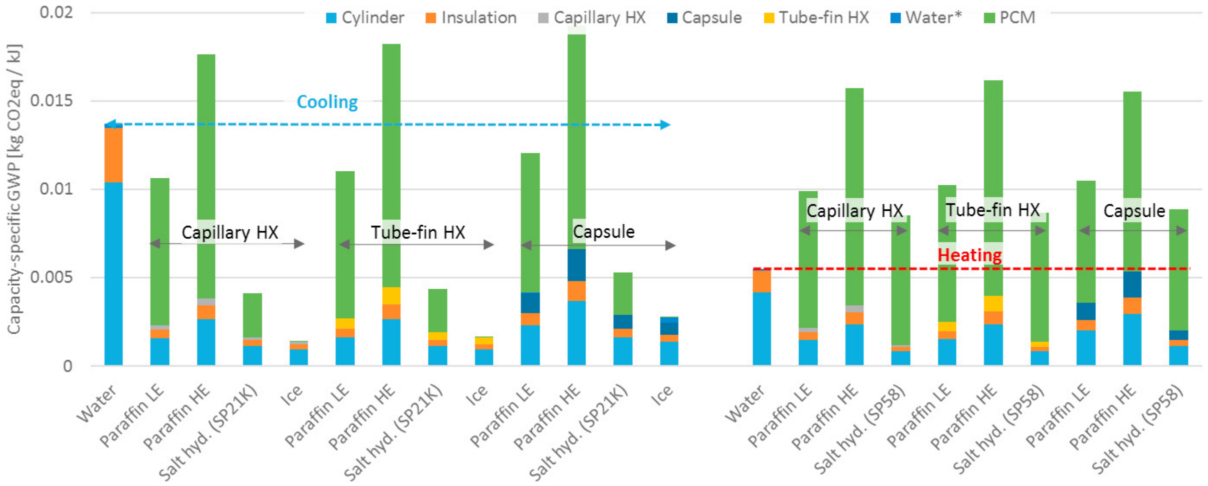

Fig. 6: GWP (left) and PENRT (right) per storage capacity of the studied configurations relative to the values of a water storage with the same configuration

2.3. Environmental evaluation of Thermochemical Storage Materials

At the current stage of the project, three classes of sorption materials have been evaluated in terms of environmental impact on material level: Silica gel, different representatives of zeolites and selected metal organic frameworks (MOFs). Their production and processing was analogously to PCMs in the LCA software suite GaBi. For materials which are not available on industrial scale yet (MOFs), it has been assumed that the synthesis takes place in medium size (batch) industrial processes. The corresponding energy and material flows have been modelled based on literature values and/or thermodynamics of the respective processes. The obtained mass specific key indicators in the impact categories considered in this study are available in the table in the appendix.

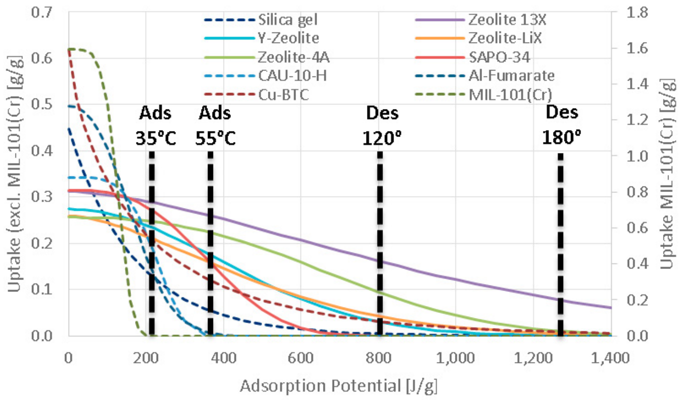

Fig. 7: Plot of the adapted Dubinin-Astakhov-Regressions used to determine the water uptake (and finally storage capacity) of the considered TCMs; the black dashed lines indicate the applicable limits of adsorption potential for the studied scenarios (listed below)

The thermal performance of the materials has been evaluated on the basis of adapted Dubinin-Astakhov-Regressions (referring to adsorbed mass instead of volume) performed on equilibrium data measured at Fraunhofer ISE (see figure 7). It has to be mentioned, that the description applied does not yield the optimal consistency with experimental data for all materials under evaluation, but was chosen for reasons of simplicity. This especially underestimates the uptake of materials with step-like isotherms (CAU-10 H, Al-Fumarate). In addition the equilibriums at high adsorption potentials, corresponding to high temperatures during desorption, may exhibit some deviations depending on the measurement principle and apparatus as well as the extrapolation of the regression.

Different scenarios are regarded:

- two desorption temperatures (T_{des}) are studied: 120°C as maximum temperature for highly efficient flat plate solar collectors and 180°C as maximum temperature for CPC evacuated tube collectors
- two adsorption temperatures (T_{ads}) are studied: 35°C (for low temperature heating, such as underfloor heating) and 55°C (assuming heat distribution via medium temperature radiators or preparation of domestic hot water)
- 10°C is assumed as evaporating and 20°C as condensing temperature (e.g. borehole)

For the reference water storage 90°C is assumed as maximum temperature, the corresponding adsorption temperature determines the lower limit of the useful temperature range.

The specific storage capacity per kg of material (c_{stor}) is calculated based on the difference in uptake between de- and adsorption (ΔX), the evaporation enthalpy of water at the adsorption temperature, the integrated adsorption potential over the working range of the material (A, see equation 2) and the sensible heat capacity. In this approximation the entropy term is disregarded:

$$c_{stor} = \Delta X \cdot h_{evap}(T_{ads}) + \int_{X_{Des}}^{X_{Ads}} A\,(X)\;dX + (T_{Des} - T_{Ads}) \cdot c_{p,sorb,60°C} \qquad (2)$$

In Figure 8, the volume specific storage density of the sorption materials is compared to water in the temperature range between the adsorption temperature and the fixed maximum temperature of 90°C. For materials with the major share of the uptake outside the operating range of the studied scenarios (CAU-10 H and Al-Fumarate for 55°C adsorption temperature and MIL-101(Cr)) the shown values are determined by the sensible heat capacity and the useful temperature difference. The remaining values range from approximately 0.7 to 3.4. As figure 7 suggested already, the useable uptake difference is far below the theoretical maximum, if the entire working range of the materials could be used for energy storage. This is the reason why the achievable energy densities are well below the theoretical values of up to 10, found in literature.

Interestingly some materials (such as Silica gel, SAPO-34 and Cu-BTC) have a higher relative storage density for the lower adsorption temperature, other hydrophilic candidates (such as 13X and 4A) show the opposite property. In the latter case, the reduction of sensible capacity of the water storage is higher than the decrease due to a lower uptake of the sorption material.

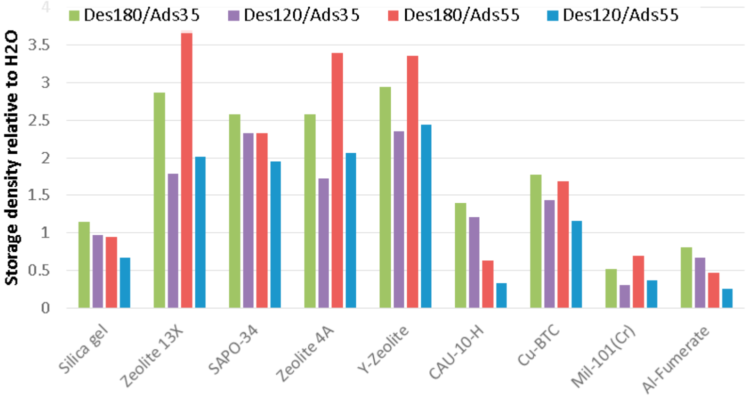

Fig. 8: Volume-specific storage density of the studied sorption materials relative to water for two des-/adsorption temperatures

Figure 9 depicts the environmental impact of a sorption storage in terms of GWP relative to water for two des-/adsorption temperatures. Values start from approximately 200 and go up to various thousands, the latter is the case for materials showing no significant uptake under the given boundary conditions. In addition, SAPO-34 has a high impact compared to water, caused by the high GWP values.

As the results for PCM showed, the evaluation on material level does not provide clear evidence of the results on component or even system level. Yet, since the integration of sorption materials into a component will further decrease the storage density due to the need for auxiliary components (especially evaporator/condenser), it is clear that a water storage constitutes a serious challenge for the environmentally beneficial use of a sorption storage. More so, since as in case of the PCMs, the presented evaluations neglects that in any application the required heat exchangers will lead to temperature gradients which will reduce the real storage density. Also, the (dis-) charging power, which is an essential characteristic of storages and directly interacts with the storage density, is not discussed at this stage.

This will be clarified in the further course of the project. In that context, two factors which favor the TCMs will also be incorporated into the analysis: a) their potential for long term storage without losses and b) the fact that most of the studied materials do not degrade during their lifetime and could thus be reused. Also the application of the materials in an open (air based) storage system may change the perspectives.

Additionally, also selected representatives of material classes such as salthydrates and liquid sorption will be looked at.

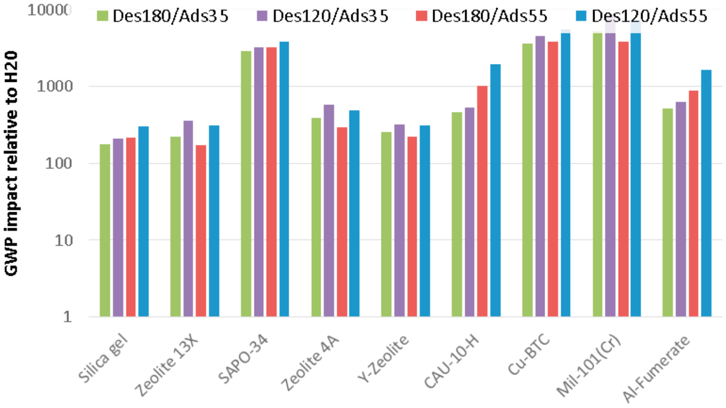

Fig. 9: Environmental impact in terms of GWP (logarithmic scale) of a sorption storage relative to water for two des-/adsorption temperatures

2.4. LCA Tool

The presented calculations are based on data, which will be publically available free of charge by the end of 2018 within an MS-Excel-based software tool. This tool will contain the environmental life cycle assessment data on material level. Besides a set of pre-configured storages, it will provide building blocks for setting up custom storage configurations and their environmental impact evaluation. Additionally, it will include an extensive database of simulation results of various storage system configurations under different boundary conditions. So the production and end-of-life data of the systems are complemented with data on their performance during useful life.

3. Conclusions

This paper gives an overview of the environmental performance of materials used for innovative heat and cold storages.

For PCM it contemplates two different levels of detail: material as well as component for a generic cooling and heating application, represented with a useful temperature difference of 6K and 15K, respectively.

- On material level, water and ice are the most beneficial storage materials from an environmental perspective, as they have a lower impact per storage capacity.
- On component level three different configurations have been studied: capillary tube and finned tube heat exchangers immersed in PCM and macroencapsulated PCM. The storage density decreases by 15% to 35% approximately; nevertheless, for the cooling application, PCM configurations with high storage density turned out favorable compared to the water storage. The reason is high environmental impact of the containment (storage vessel) and insulation, which is the same for all configurations and is used inefficiently in case of water as sensible storage medium.

Sorption materials have been studied for heat storage in a solar thermal application. The analysis of the material characteristics insinuate that the achievable storage density relative to water in this application is much lower than typical theoretical values presented in literature (0.5 to 2.5 instead of ~10), even though required auxiliary components are not yet considered. The environmental impact in terms of GWP caused by the material production is at least 260 times higher per unit of stored energy for the considered scenarios. Analysis on component and system level is still pending but it can be anticipated that the perspectives of this technology are rather restricted.

These results must be interpreted knowing that they are based on simplified calculations of ideal storages, ignoring heat losses and temperature gradients and the like.

A software tool will be publically available for free, which will allow the user to study custom storage configurations in terms of environmental impacts. Additionally, it will include an extensive database of simulation results of various storage system configurations under different boundary conditions. So the production and end-of-life data of the systems are complemented with use phase data, providing an environmental assessment of the systems life cycle.

Acknowledgements

The authors acknowledge the financial support initially by the German Federal Ministry for Economic Affairs and Energy for the Project “Speicher-LCA” (Grant number: 03ET1333). The authors furthermore thank the company Rubitherm GmbH for providing specific data on the production of various PCM materials and encapsulation.

Appendix A. Material properties and LCAI values used for calculations

Material	**specific heat capacity***	**Melting enthalpy**	**density**	**GWP**	**PE**
	kJ/kg/K	**kJ/K**	**kg/m3**	**kg$_{CO2eq}$ / kg**	**MJ/kg**
Paraffin LE	2	150	770	2.1	31.2
Paraffin HE	2	250	770	2.1	31.2
Salt hyd. Cooling (SP21EK)	2	180	1400	0.5	6.2
Salt hyd. Heating (SP58)	2	250	1300	2.0	29.5
Ice	3.21	333.5	918	0.01	0.06
Water	4.19	0	1000	0.01	0.06
25% Ethylenglycol-Water	3.7	0	1028	1.1	35.7
PP	1.7	0	946	1.3	58.9
Aluminum	0.90	0	2710	0.9	14.0
Copper	0.39	0	8940	1.1	23.1
HDPE	1.9	0	963	1.2	40.2
Silica gel	1.04	-		2.3	19.6
Zeolite 13X	1.68	-		5.5	70.6
SAPO-34	1.42	-		70.3	1058.4
Zeolite 4A	1.03	-		8.7	100.1
Y-Zeolite	1.72	-		6.0	70.3
CAU-10-H	1.59	-		8.5	155.0
Cu-BTC	1.30	-		69.9	1897.4
Mil-101(Cr)	1.16	-		22.9	568.7
Al-Fumerate	1.67	-		8.0	123.5

* Values of specific heat capacity for adsorbents are temperature dependent; the considered values refer to 60°C

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