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ORIGINAL ARTICLE

Life cycle inventory and performance analysis of phase change materials for thermal energy storages

Naveenkumar Madeswaran[1] · Fenil J. Desai[1] · Eylem Asmatulu[1]

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Abstract
Solar energy is a renewable energy that requires a storage medium for effective usage. Phase change materials (PCMs) successfully store thermal energy from solar energy. The material-level life cycle assessment (LCA) plays an important role in studying the ecological impact of PCMs. The life cycle inventory (LCI) analysis provides information regarding the material and energy requirements and economy of PCMs. This work presents an estimated LCA and LCI values in order to reveal all the mentioned effects of PCMs on storing thermal energy generated by concentrated solar thermal power plants. The goal of this study was to provide guidance for PCM system design based on a matrix that considers the performance, costs, and environmental impact. The ecoinvent global database (version 3) was used for the life cycle inventory analysis. For this study, PCMs were selected based on physical and chemical properties as well as state and melting temperatures (300–500 °C) that are suitable for charging and discharging a large amount of thermal energy. The performance of PCMs was determined based on their thermal effusivity. Results indicate that compared to other PCMs, sodium nitrate (100%) used less heat energy, but when comparing the amount of electricity usage for PCM compounds, potassium nitrate (65.31%) + potassium carbonate (34.69%) used less electricity. From the emissions data for PCMs from raw materials to factory gate (cradle-to-gate), Na_2CO_3 produced the lowest emissions to air, although harmful emissions to water. The performance of PCM mixtures was better, with thermal conductivity almost 3.5 times higher than that of individual PCMs. However, the cost of PCM mixtures was three times higher than that of individual PCMs. This comprehensive compilation of PCM data can be very helpful in the selection of a suitable PCM while offering a fine balance between cost and performance.

Keywords Life cycle analysis · Life cycle inventory analysis · Phase change material · Carbon footprint · Emissions

1 Introduction

Thermal energy storage (TES) technologies have a greater potential to reduce the gap between energy generation, utilization, and peak energy demand [24, 39, 42]. Thermal capacity and operating temperature range are two considerations in deciding the type and design of any thermal storage system. TES has multiple applications, such as a heat pump, which could be used for heating in winter and cooling in summer [10, 36, 46]. TES is mainly classified into sensible, latent, and thermochemical energy systems. Sensible TES stores and releases energy without changing the phase of the material [12, 15, 42]. There is no phase change feature in the sensible storage system, and only the temperature of the storage medium increases or decreases during the thermal storage process. In contrast to sensible heat storage, the energy storage density of phase change material (PCM) is much higher. PCM absorbs or releases a large quantity of latent heat energy as it changes its physical condition, i.e., from solid to solid, solid to fluid, fluid to gas, and vice versa [28, 29]. The phase change occurs when the material reaches the transition temperature in a heating or cooling process. The major benefit of PCM is that its temperature remains stable during latent heat

Highlights
1. PCMs were selected based on physical, chemical and thermal properties.
2. The performance of PCMs was determined based on their thermal effusivity.
3. LCI of PCMs was performed using the cradle-to-gate approach.
4. The material-level LCA is important for understanding environmental impact of PCMs.
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✉ Eylem Asmatulu
eylem.asmatulu@wichita.edu

1 Department of Mechanical Engineering, Wichita State University, 1845 Fairmount, Wichita, KS 67260, USA

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absorption or release. The major drawbacks of PCM are its lack of thermophysical properties, low thermal conductivity (0.15–0.3 W/mK), lower cyclic stability, phase isolation, variable melting, change in volume, and high cost.

Some specific materials, such as paraffin, salt hydrates, fatty acids, and sugar alcohols, are common PCMs and have good enthalpy of fusion, suitable phase change temperature, cyclic stability, and good thermal conductivity [41]. However, each PCM material has varying characteristics, and to use a specific PCM, it is necessary to study and understand its performance [33]. Eco-Indicator 99 is one of the methods used to calculate the environmental effects on human health, energy consumption, and biodiversity. To study all of these parameters, a life cycle analysis (LCA) was developed to provide insight into the number of compounds emitted from raw materials to the manufacturing phase to the customer [5, 8]. PCMs are selected based on several criteria such as melting temperature, latent heat of fusion, specific heat, thermal conductivity, thermal expansion coefficient, toxicity, flammability, and cost.

Kyriaki et al. [25] investigate PCMs for thermal applications by considering environmental (relying on the life cycle analysis approach) as well as economic performance (based on the life cycle cost analysis technique) measures, but omitting solar power generation applications. Many studies have emphasized that to limit the general natural effect, the utilization of PCMs and the valuable usage of the buildings should be improved, while new PCMs with less environmental effect should be created. Considering the environmental impact of PCMs utilized in both heating and cooling systems, it was noted that the environmental impact was considerably decreased when PCM systems were utilized in conjunction with conventional gas or oil systems. Based on life cycle cost analysis, PCMs are not economically viable due to their high initial investment cost [25].

In research conducted by Mahfuz et al. [27], shell and tube thermal energy storage systems utilizing paraffin wax are employed in a water heating system to investigate its performance for solar water heating application. They conducted a cost analysis for thermal energy storage systems by including both energy and exergy. Furthermore, the total life cycle cost was computed for various flow rates of the heat transfer fluid (HTF). As a result, with the 0.033 kg/min and 0.167 kg/min flow rates of water being an HTF, energy efficiencies were noted as 63.88% and 77.41%, respectively; however, in exergy analysis, efficiencies were noted as approximately 9.58% and 6.02%, respectively. Considering the total life cycle cost, the flow rate was about $654.61 for 0.033 kg/min, which was lowered to $609.22 by increasing the flow rate to 0.167 kg/min. Thus, it can be concluded that the total life cycle cost can be decreased by increasing the flow rate [27].

Johansson and Norrman [21] compared three different phase change materials (octadecane, xylitol, and manganese nitrate hexahydrate) used for thermal energy storage systems in terms of environmental, health, and safety aspects. To conduct the LCA, they considered the cradle-to-grave life cycle boundary for a thermal energy storage heating system running in Scandinavian environments presuming 52 cycles per year. Results show that octadecane is desirable with respect to the global warming potential for more than 100 years (ca 4.5 kg CO_2/kg octadecane produced), and xylitol is more desirable with respect to cumulative energy demand (ca 21.5 MJ per kg xylitol produced) as well as energy payback time (1.17 years). Considering the health and safety aspects, xylitol is the most promising material [21].

Oró et al. [34] compared the environmental impact of three different thermal energy storage systems for solar power plants. To establish the LCA, they developed systems including sensible heat storage in both solid (high temperature concrete), liquid (molten salts) thermal storage media, and latent heat storage, which utilizes PCMs. Their purpose was to determine if the energy savings associated with the stored energy of the different systems was sufficient to balance out the environmental impact generated throughout the manufacturing as well as operation phase of each storage system. Of all the systems, those relying on solid media exhibit the lowest environmental impact per kWh stored; however, the liquid media exhibits the highest impact per kWh stored since it requires more material and intricate equipment [34].

Velraj et al. [43] determined the performance of PCMs by evaluating their thermal conductivity since thermal conductivity is directly proportional to the efficiency of the respective PCM. They found that the initial volume of the PCM should not be more than 80% of the capsule volume when using a rigid capsule and that the finned tube method was simple and cheap [43]. Jegadheeswaran and Pohekar [20])stated that using multiple PCMs with different melting points was the most effective material for thermal heat storage. However, the heat transfer values of some of those materials and methods with a single PCM became poor due to the variable decrease in the flow direction of the heat transfer fluid [20]. Williams et al. [45] announced that the elements with low atomic numbers have better thermal performance than others. They evaluated several fluorides for a next-generation nuclear plant and nuclear hydrogen initiate (NHI) plant and found that chloride salts also met the chemical stability and high-temperature requirements. They ranked the chloride and other salts based on corrosion characteristics, but the results were inconclusive. Among all other salt components, nitrate salts have a high melting point and high heat capacity [45].

PCMs are utilized in various business applications including energy storage and temperature stabilizations (cooling of phone switching boxes, heating pads, and clothes). The greatest potential market is mainly for heating and cooling of building. Nonetheless, these captivating materials have recently been rediscovered and employed for a broad scope of advance technologies, such as smart drug delivery, information storage, barcoding, and detection [19]. The biocompatible and degradable PCMs, such as fatty acids and fatty alcohols, could empower temperature-regulated drug delivery framework. Distinctive diffusivity of the medication in solid and fluid PCMs permits the framework to effectively contain a medication at a temperature under the melting point and release the medication when needed. Also, incorporating quantum dots of various semiconductors could offer luminescent properties for PCMs which make them useful as a probe for biological imaging. Moreover, encapsulation in a PCM could provide another methodology for fine-tuning the emission energy of a quantum dot, in which the energy can be precisely controlled through the nearby strain related with the volume change of the PCM. This is a main resource in quantum communication and quantum information processing (Hunam et al., 2014).

Studies have concluded that LCA can be a very useful method to identify and provide an opportunity to enhance the environmental performance of a product or service [2, 3, 30, 35]. This can eventually help governments and industries select a system or service based on specifics such as emissions data and the long-term effect of ecological performance. The major stages of LCA are defining the goal and scope, life cycle inventory (LCI) analysis, impact analysis, and data interpretation [6]. The important phase of the LCA is the LCI because it allows one to calculate the total amount of electrical energy, heat energy, material input and output of a component, and ecological impact during a product's or service's lifetime or partial lifetime (i.e., cradle-to-grave or cradle-to-gate). These factors help to select suitable PCMs based on customer and user requirements. The LCI is widely used to compile reports based on carbon dioxide emissions from a material [16, 17]. The major drawback of this method is obtaining accurate LCI data for PCMs and other parameters for performance calculations. The LCI is a direct accounting of all systems of interest involved, and it tracks the details of all energy types by the LCI assessment of water, air, emissions to water and air, and all flows in and out of the product system, including raw resources and materials, by specific substances. The disadvantage here is that because of the overarching approach, the LCI analysis requires a considerable amount of time for compiling several datasheets, conducting elaborate experiments, and selecting a PCM suitable for customer needs, thereby making the process more complex [9, 32]. To overcome this, a study was performed for LCI analysis on bioenergy, imported fuels, modern biogas plants, and organic rapeseed based on data from the ecoinvent database to investigate the energy products from biomass. This study examined the process in three segments: the first being the production and use of biogas, methanol, plant oils, and ethanol, followed by the second involving biofuels import data (transportation data),and the third focusing on the minimization of methane emissions by covering the storage of the modern biogas plant. Results were calculated based on the ecoinvent database, which is available online, and it was concluded that this tool could be useful for calculating the LCI. Since 2003, the ecoinvent database has empowered organizations to fabricate items to be more in agreement with nature, policymakers to actualize new strategies, and purchasers to embrace more earth eco-friendly behavior [1].

The objective of this paper is to generate a detailed set of LCI data for selected PCMs. The key goal here is to assess, compare, and analyze LCI data along with the cost and performance of PCMs for the purpose of selecting a suitable PCM for a concentrated solar power plant application. The LCI is performed from cradle-to-gate, in order to reduce the complexity of performing the LCA. Figure 1 shows the cradle-to-gate life cycle boundary of PCMs. This type of analysis could be effective for environmental product declaration (documented information about environmental and health impacts) and is important in providing customers with knowledge about the material in order to make better choices. In this report, the ecoinvent version 3 database is used to gather the LCI data for respective PCMs and PCM mixtures [26].

The novelty of this study is that for the first time we provide the major life cycle impact and inventory analysis of the PCMs for solar energy storage systems, which is necessary to make a scientific evaluation on the cost, materials performance, and environmentally friendliness. This scope extends to help readers, customers, designers, and manufactures to have comprehensive understanding about the materials and their properties for better materials selections, which have not been studied by engaging with the cradle-to-gate LCI analysis for PCMs. The fundamental knowledge and skill gained in this study will be used to develop high-performing energy storage systems in the future.

2 Materials and methodology

2.1 Selection of materials

The basic properties of various PCMs, such as energy storage density, cyclic stability, operating temperature, and reaction enthalpy, are selected to perform LCA analysis, and these are provided in Table 1. These PCMs were selected based on their composition and invariant temperature, which includes eutectic, peritectic, and melting temperature; specific heat capacity; and latent heat of fusion. Based on the required temperature range, melting point, and enthalpy, sodium nitrate ($NaNO_3$), potassium

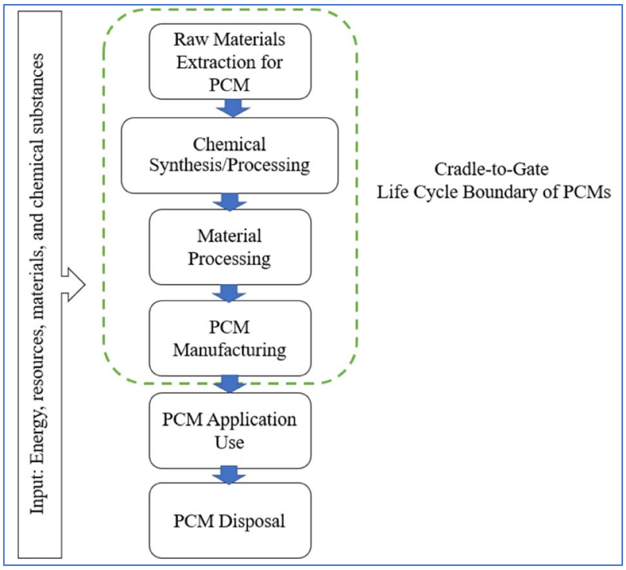


Fig. 1 Cradle-to-gate life cycle boundary of PCMs

nitrate (KNO_3), and potassium hydroxide (KOH) are the only salt candidates that fulfill all requirements.

2.2 LCI analysis

The LCI data for PCMs and PCM mixtures were calculated using the ecoinvent database 3 because it has more international scope [44]. This database enables the inventory of each specific goods for performing LCA analysis and to complete supply chains. Data were collected for individual compounds and then calculated for binary and ternary mixtures based on their composition. LCI analysis includes electricity used, heat energy required, and emissions generated (to air and water) and was calculated based on the annual production of PCMs.

2.3 Performance analysis

Performance analysis was used to study the eco-friendliness and thermal characteristics of possible PCMs. It provides detailed characteristics to select a range of PCMs based on operating temperature and heat requirements [22, 31, 38]. Ample amounts of charging/discharging thermal energy are produced during the melting and solidifying PCMs at their transition temperatures with surroundings. To calculate the thermal performance, thermal inertia and thermal effusivity were considered [11]. High thermal effusivity makes PCMs possible to activate thermally faster, thus storing more thermal energy during the energy storage/usage process. The higher thermal effusivity of PCMs enables it to absorb and release thermal energy in a rapid manner. Thermal effusivity of the PCM is calculated as [11]:

$$e = \left(k \times \rho \times C_P\right)^{\frac{1}{2}} \tag{1}$$

where e is the thermal effusivity, ρ is the density, Cp is the specific heat capacity, and k is the thermal conductivity ($W.s^{1/2}/m^2$). One study on molten salts described a formula to calculate the thermal conductivity of binary salts [11]. The thermal conductivity for a binary PCM compound is given as:

$$\lambda_{bi} = \lambda_A \times \left\{ \left[1 - \tau^2\right] + \left[\frac{\tau^2}{1 + \left(\frac{\lambda_A}{\lambda_B} - 1\right) \times \frac{\tau}{2}} \right] \right\} \tag{2}$$

where λ_{bi} is the thermal conductivity of the binary PCM compound, λ_A is the thermal conductivity of compound A,

Table 1 Parameters of PCMs [25, 26]

Series No	System components (weight percentage)	Melting point (mp)/ eutectic (E) (°C)	Cp, J/g.K		ΔH_m, J/g
			Solid	Liquid	
1	$NaNO_3$ (100.00)	mp306	1.859	1.830	178.560
2	KNO_3 (100.00)	mp335	1.439	1.480	100.190
3	KOH (100)	mp360	–	1.481	–
4	KCl (7.18) + KNO_3 (92.82)	E307.87	1.156	1.177	105.630
5	KNO_3 (65.31) + K_2CO_3 (34.69)	E325.73	0.812	0.832	71.580
6	KNO_3 (91.15) + KBr (8.85)	E329.84	1.161	1.161	100.930
7	Na_2CO_3 (56) + Li_2CO_3 (44)	E487	–	1.380	368.000
8	KCl (54.75) + LiCl (45.25)	E352.53	1.009	1.279	267.960
9	K_2CO_3 (22.05) + KOH (77.95)	E365.5	1.332	1.394	164.350
10	K_2SO_4 (16.54) + KOH (83.46)	E376	1.329	1.408	174.090
11	KBr (47.74) + LiBr (52.26)	E327.8	0.562	0.672	333.050
12	Na_2CO_3 (37) + K_2CO_3 (35) + Li_2CO_3(28)	E397	–	1.602	34.760

Eutectic = mixture of compounds with higher freezing point than water.

λ_B is the thermal conductivity of compound B, τ is the density fraction, ρ_A is the density of compound A, ρ_B is the density of compound B, W_A is the weight of compound A, W_B is the weight of compound B, and the unit of thermal conductivity is given as W/m–K and τ:

$$\tau = \left(\frac{2 \times \frac{\rho_A W_B}{\rho_B W_A}}{1 + \frac{\rho_A W_B}{\rho_B W_A}} \right)^{1/3}$$

The density of a binary compound is given as [46]:

$$\frac{1}{\rho_{bi}} = \frac{W_A}{\rho_A} + \frac{W_B}{\rho_B} \tag{3}$$

where ρ_{bi} is the density in kg/m^3 of the binary PCM compound.

2.4 Energy usage and emission calculation

Energy and emissions data for PCMs from raw materials to factory (cradle-to-gate) was calculated using the ecoinvent version 3 commercial database. The energy and emissions data targets show researchers how the combination of salt hydrates can impact the required energy usage and emissions generated during the production and usage of PCMs. The amount of energy used during the production of 1 kg of PCM was taken as the reference to calculate the total energy usage for PCMs and PCM mixtures. The environmental assessment was done to show emissions generated at material level using data available from the ecoinvent 3 database. A comparative study of PCMs and their combination was performed to study the emissions to air and water. The emissions to air help to understand the impact on the environment, as these greenhouse gases largely contribute to the global warning. The US Environmental Protection Agency TRACI method available in the Athena IE software was used to study the environmental impact analysis (Athena Impact Estimator for Buildings, 2014). The emissions results generated by Athena IE are reported for end-of-life phases of the life cycle.

2.5 Cost analysis of raw materials

Cost data was determined using Lab Alley, a lab chemical and equipment supplier, in order for it to be comparable to all compounds because they are obtained from the same vendor [25]. The cost of the material depends on the overall cost of production, existence of raw materials, and demand for the material. Cost analysis for each PCM was performed based on its purchase price since this research mainly focused on selection of the materials by customers [25]. Lab Alley has a competitive price range and an abundant selection of compounds; therefore, Lab Alley was used for the cost analysis.

2.6 Precision and accuracy

In LCI analysis, 12 compounds were considered, out of 8 are compared based on the heat energy usage data (from the ecoinvent database) while the remaining 4 compounds are compared based on other parameters, including melting temperature, heat of fusion, density, specific heat capacity, thermal conductivity thermal effusivity, and cost, since some of the heat energy usage for the respective compounds are unavailable. Performance analysis is conducted by calculating thermal effusivity at the highest melting point among the selected compound (500 °C) since it defines the charging ability of the respective PCMs. After comparing the compounds for LCI, performance and cost analysis data and emission analysis (emission to air and emission to water) were performed for the top 3 compounds based on performance that will also analyze the environmental impact values taken from ecoinvent database. Table 2 explains the LCI, performance, and cost analysis of PCMs. The exact combination (65.31%/34.69%) of these compounds could make synergistic effects (eutectic behavior with lower melting point) which can reduce amount of the electricity for the heat energy storage.

3 Results and discussion

3.1 LCI analysis

Data from the life cycle inventory analysis of the PCMs obtained from the ecoinvent version 3 are given in Table 3. The most common salt hydrates and metallic alloys, such as $NaNO_3$, KNO_3, KOH, K_2CO_3, KCl, LiCl, Li_2CO_3, KOH, K_2SO_4, NaCl, and Na_2CO_3, were used to create a simple database [13]. This database shows the amount of annual production of each PCM, the energy and heat used for production, and the emissions generated during the process.

3.2 Performance analysis

3.2.1 Thermal effusivity

Thermal effusivity was calculated to determine the performance of individual phase change materials and PCM mixtures. Thermal conductivity, density, and specific heat capacity of the PCMs and PCM mixtures were obtained from the Knovel database (engineering data and technical references), which provides chemical and physical properties of several materials (Knovel Corporation, 2019). Thermal performance was calculated for the liquid specific heat

Table 2 LCI, performance, and cost analysis of PCMs

PCM	Inventory analysis		Performance	Cost
	Heat energy MJ	Electricity kWh		
$NaNO_3$ (100%)	2.00	0.33	1545.40	11.00
KNO_3 (100%)	4.56	NA	1217.90	14.40
KOH (100%)	7.34	1.86	1253.10	28.10
KCl (7.18) + KNO_3(92.82)	4.51	NA	1096.00	14.70
KNO_3 (65.31%) + K_2CO_3 (34.69%)	3.67	0.12-NA	1089.20	15.80
KNO_3 (91.15%) + KBr (8.85%)	4.15-NA	NA	1133.50	16.20
Na_2CO_3 (56%) + Li_2CO_3(44%)	6.17	0.28	2605.20	39.10
KCl (54.75%) + LiCl (45.25%)	2.12-NA	0.26-NA	1154.10	77.80
K_2CO_3 (22.05%) + KOH (77.95%)	6.16	1.52	878.50	26.00
K_2SO_4 (16.54%) + KOH (83.46%)	7.08	1.57	566.10	24.90
LiBr (52.26%) + KBr (47.74%)	NA	NA	1104.10	107.50
Na_2CO_3 (37%) + K_2CO_3 (35%) + Li_2CO_3 (28%)	4.73	0.29	2781.50	33.10

capacity using MATLAB. Thermal conductivity is measured using C-Therm, a thermal conductivity analyzer that can directly measure the thermal effusivity of compounds. This analyzer uses a modified transient plane source, and it agrees with current standards (C-Therm Technologies Ltd., 2019). Researchers consider C-Therm to be a beneficial device because it reduces considerable time and errors that occur by assuming the density and thermal conductivity of the materials. Thermal effusivity that was calculated using the C-Therm for each individual PCM and their mixtures showed that a combination of three PCMs had the highest thermal conductivity and better thermal effusivity, hence better performance. The binary compound mixture also shows better thermal effusivity and conductivity compared to individual salts, as shown in Table 4. The good agreement indicates that better thermal effusivity increases the volumetric heat capacity and helps to improve overall performance of the PCMs by exchanging the surrounding heat.

A mixture of three PCMs (C12) showed the highest performance compared to other PCMs. This proves that a combination of PCMs has higher performance than a single PCM, which also proves that among single-compound PCMs, those with nitrate had a higher performance than other single compounds. The performance of PCMs in terms of thermal effusivity is shown in Fig. 2. Density and thermal conductivity of the ternary compound are also higher than that of single or binary compounds, as shown in Table 4. Thermal conductivity of the PCMs helps during energy absorption and release and remains constant for individual and binary PCMs, as shown in Table 4. However, a combination of carbonate PCMs showed sudden improvement in thermal conductivity. The specific heat capacity of the ternary PCM (C12) compound was 1602 kJ/gK and for sodium nitrate (C1) was 1830 kJ/gK. Although the specific heat capacity of sodium nitrate is higher than the ternary compound, the thermal conductivity of the ternary compound is almost 3.5 times higher than sodium nitrate. Each PCM has its own advantages and disadvantages, such as cost.

3.3 Energy usage

Depending on data from the ecoinvent version 3 database, pure sodium nitrate uses less heat energy than others from gate-to-gate and is followed by a combination of potassium nitrate and potassium carbonate (C5). However, the amount of electricity usage for the respective compound C5 uses less electricity and is followed by the ternary PCM (C12). Since the energy usage data for some material are unavailable, the comparison was based on other parameters from the selection criteria. Figure 3 shows the heat energy and electricity used by 1 kg of each PCM from cradle-to-gate. Based on the results, the total energy usage is given in Table 5, which shows that pure sodium nitrate uses less energy than other compounds and is followed by a combination of potassium nitrate/potassium carbonate and then the ternary salt mixture (C12).

3.4 Emissions

As can be seen in Fig. 4, data showing the emissions to air indicate that sodium nitrate emits carbon dioxide during production, which impacts the environment in several ways, including causing a greenhouse effect, climate change, and acid rain. Sodium carbonate emits a small amount of ammonia, 0.37 kg, during production. Ammonia in the air causes nose, eyes, and throat irritation as well as skin burns. Lithium carbonate emits carbon dioxide and nitrogen. Nitrogen emission to the air causes respiratory problems. In Fig. 4, the value of water and particulate < 2.5 µm is 4.2×10^{-7}, so it is negligible and not visible in present figure. In European countries, 21% of nitrogen emission is due to energy production. As can be seen in Fig. 5, data showing the emissions

Table 3 LCI Data of PCMs

Series No	Material	Inventory (Reference product = 1 kg)	Emissions to Air	Emissions to Water
1	$NaNO_3$	Total annual production = 100,000,000 kg Electricity used in process = 0.3330 kWh Heat energy used in process = 2 MJ	Carbon dioxide = 0.5177 kg	Carbonate = 0.0372 kg Nitrate = 0.0384 kg Sodium ion = 0.0285 kg
2	KNO_3	Total annual production = 500,000,000 kg Heat energy used in process = 4.5600 MJ	–	–
3	K_2CO_3	Total annual production = 320,000,000 kg Electricity used in process = 0.3330 kWh Heat energy used in process = 2 MJ Potassium hydroxide used in process = 0.8543 kg	Carbon dioxide = 0.0168 kg Water = 0.0093 m^3	Hydroxide = 0.0130 kg Potassium ion = 0.0297 kg Water = 0.0147 m^3 Sodium ion = 0.0285 kg
4	KCl	Total annual production = 32,800,000,000 kg Solid waste = 0.0007 kg Hazardous waste = 0.0003 kg Diesel used in process = 0.1390 MJ Heat energy used in process = 3.7288 MJ	Hydrogen chloride = 9.28×10^{-6} kg Particulates < 2.5 um = 7.7×10^{-7} kg Particulates > 10 um = 1.4×10^{-5} kg Water = 0.0063975 m^3	Chloride = 0.1260 kg Magnesium = 0.0121 kg Sodium ion = 0.0736 kg Sulfur = 0.0125 kg Calcium ion = 0.0021 kg Potassium ion = 0.0016 kg Water = 0.0102 m^3
5	LiCl	Total annual production = 7,200,000 kg Electricity used in process = 0.5694 kWh Lithium carbonate used in process = 0.9273 kg Hydrochloric acid used in process = 0.9023 kg	Carbon dioxide = 0.5238 kg Hydrogen chloride = 0.0018 kg Water = 0.0093 m^3	Carbonate = 0.0376 kg Chloride = 0.0421 kg Lithium ion = 0.0088 kg Total organic carbon = 0.0174 kg Water = 0.0147 m^3
6	Li_2CO_3	Total annual production = 148,080,296 kg Hazardous byproduct waste = 0.0002 kg Electricity used in process = 0.5800 kWh Heat energy used in process = 2.9635 MJ Diesel used in process = 1.8800 MJ	–	–
7	KOH	Total annual production = 132,236,940,655,721 kg Salt tailing from potash mine = 0.023 kg Electricity used in process = 1.8601 kWh Heat energy used in process = 7.3420 MJ Potassium chloride used in process = 0.4930 kg	Water = 0.0013 m^3	Chloride = 0.038 kg Potassium ion = 0.013 kg Water = 0.0031m^3
8	K_2SO_4	Total annual production = 864,367,816,091,954 kg Electricity used in process = 0.1220 kWh Heat energy used in process = 5.7600 MJ Potassium chloride used in process = 1.0300 kg Sulfuric acid used in process = 1.1300 kg	Particulates < 2.5 um = 1.19×10^{-8} kg Particulates > 10 um = 3.76×10^{-8} kg	–
9	NaCl	Total annual production = 132,236,940,655,721 kg Non-hazardous byproduct waste: Decarbonizing waste = 0.03 kg Wastewater = 0.0038 m^3 Electricity used in process = 0.17 kWh Heat energy used in process (industrial) = 0.1970 MJ Diesel used in process = 0.0043 MJ Soda ash used in process = 0.0127 kg	Water = 0.0018 m^z	Water = 0.0047 m^3

Table 3 (continued)

Series No	Material	Inventory (Reference product = 1 kg)	Emissions to Air	Emissions to Water
10	Na_2CO_3	Total annual production = 17,403,250,754,717 kg Heat energy used in process = 7.22 MJ Non-hazardous byproduct waste: Calcium chloride = 1.0500 kg Inert waste = 0.2500 kg Electricity used in process = 0.0400 kWh	Ammonia = 0.0020 kg Water = 0.0406 m^3	Cadmium = 1.73×10^{-7} kg Calcium = 0.1000 kg Chloride = 0.2400 kg Copper ion = 1.65×10^{-6} kg Lead = 1.49×10^{-5} kg Mercury = 1.75×10^{-9} kg Nickel ion = 1.15×10^{-6} kg Nitrogen = 0.0002 kg Phosphorus = 5.21×10^{-5} kg Solid inorganics = 0.0993 kg Water = 0.0656 m^3

Table 4 Performance of PCMs

PCM No	PCM components (weight percentage)	Compound density (Kg/m^3)	Compound thermal conductivity (W/m·k)	Performance (thermal effusivity) ($Ws^{1/2}/m^2K$)
C1	$NaNO_3$ (100.00)	2260.00	0.58	1545.40
C2	KNO_3 (100.00)	2110.00	0.48	1218.43
C3	KOH (100)	2120.00	0.50	1253.10
C4	KCl (7.18) + KNO_3 (92.82)	2100.10	0.47	1076.00
C5	KNO_3 (65.31) + K_2CO_3 (34.69)	2211.00	0.64	1089.20
C6	KNO_3 (91.15) + KBr (8.85)	2154.40	0.51	1133.50
C7	Na_2CO_3 (56) + Li_2CO_3 (44)	2331.00	2.11	2605.30
C8	KCl (54.75) + LiCl (45.25)	2019.70	0.52	1154.10
C9	K_2CO_3 (22.05) + KOH (77.95)	2181.40	0.25	878.50
C10	K_2SO_4 (16.54) + KOH (83.46)	2193.70	0.10	566.10
C11	KBr (47.74) + LiBr (52.26)	3080.30	0.54	1058.50
C12	Na_2CO_3 (37) + K_2CO_3 (35) + Li_2CO_3 (28)	2367.40	2.04	2781.50

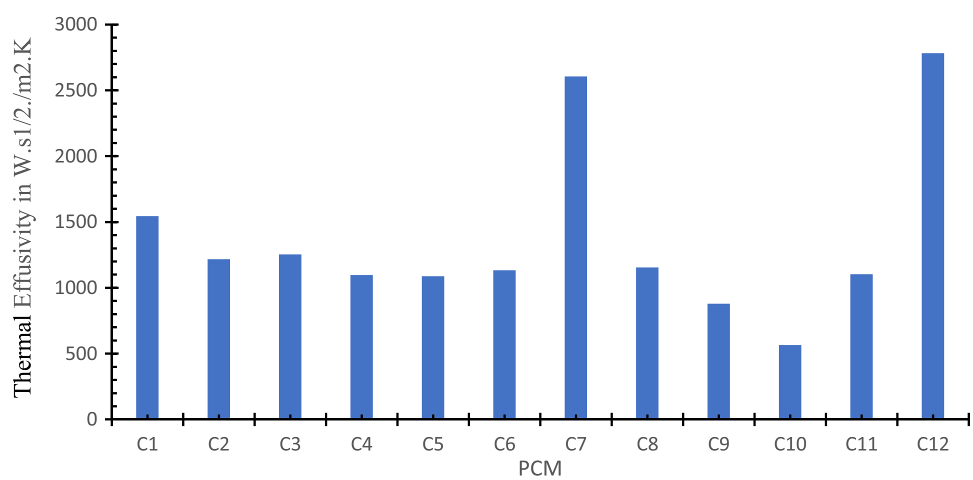


Fig. 2 Performance data for PCMs

Fig. 3 Energy usage data for PCMs

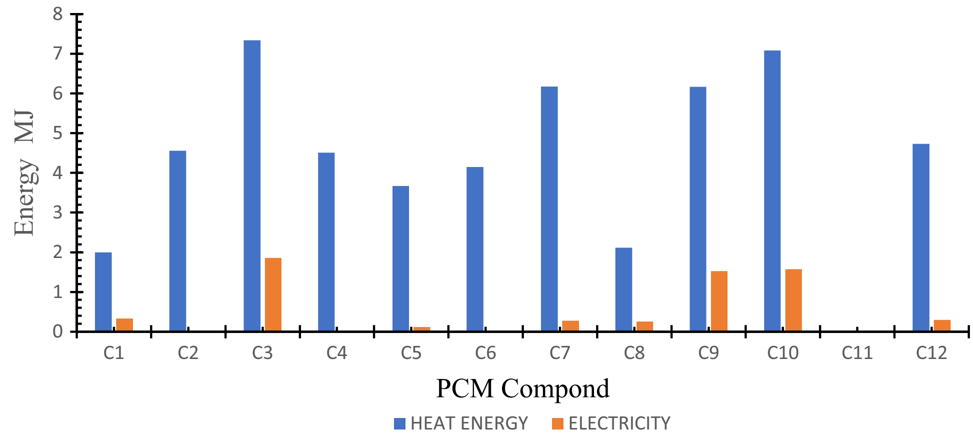


Table 5 Total energy usage

PCM	Energy usage (MJ)
$NaNO_3$ (100%)	3.199
KNO_3 (65.31%) + K_2CO_3 (34.69%)	4.088
Na_2CO_3 (37%) + K_2CO_3 (35%) + Li_2CO_3 (28%)	5.785

to water indicates that sodium nitrate uses 0.024 m^3 of water from the environment for cooling. Sodium carbonate also emits a small amount of cadmium ion, copper ion, lead, mercury, nickel ion, nitrogen, and phosphorous and uses 0.04024 m^3 of water from the environment for cooling. Emissions data for composition Nos. C2, C6, and C11 were not available.

The amount of emissions produced during the production of each PCM compound is shown in Table 6 Emissions data is discussed based on the harmful gases emitted by a PCM from the raw material-to-production phase. Emissions data clearly show the potential environmental impact of PCMs during production, use, and end of life. These data indicate the intuitive aggregated potential environmental impacts due to emissions to air and water.

3.5 Cost analysis

The cost of PCMs is also one of the major factors in the selection for long-term applications. It can be seen that the mixture of three PCMs (C12), the ternary compound, costs three times the amount of a single compound and has 1.8 times better performance compared to sodium nitrate. Lab Alley data show that a single-compound PCM costs less than a mixture of various PCMs, as shown in Fig.6. It was noticed that bromide-based compounds cost more than the other compounds. The price of PCMs primarily depends first on the raw materials and then on the encapsulation required to prevent the contamination of PCMs by the environment, energy storage density, cyclic stability, and temperature

Fig. 4 Emissions to air

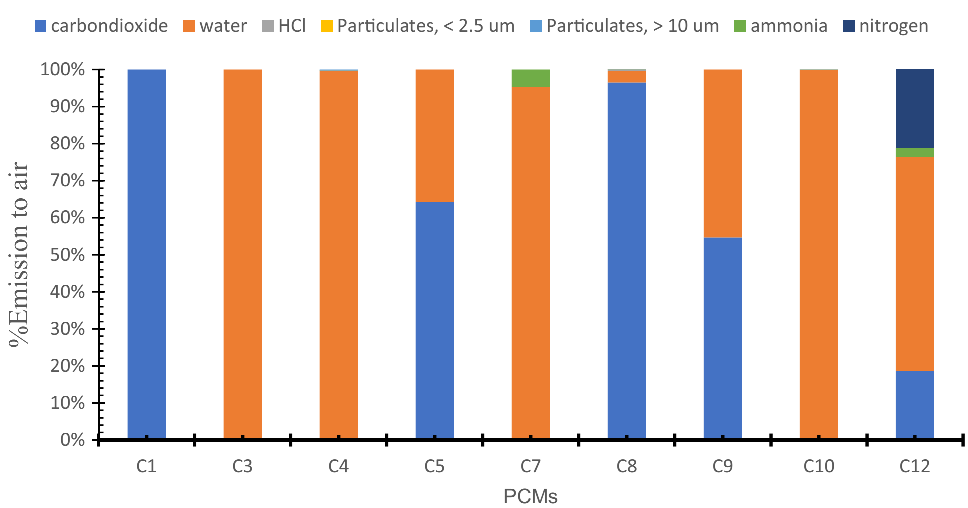
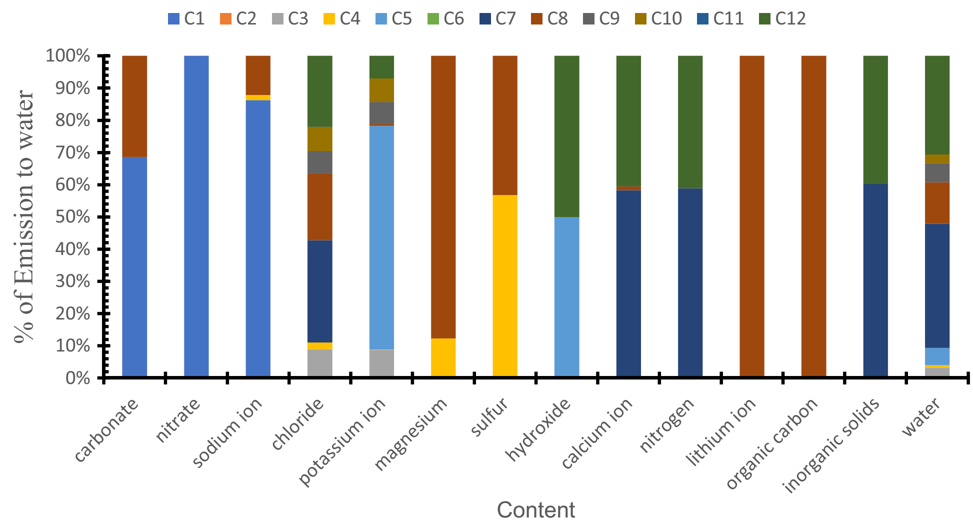


Fig. 5 Emissions to water



range of the PCMs. The cost considered in this study is for pure laboratory-grade PCMs, which generally cost more than commercial-grade PCMs.

4 Conclusions

Most of the recent studies on phase change materials are based on selecting suitable components. However, there are no simple methods for doing this. PCM selection is the process by which several parameters, such as density, thermal conductivity, latent heat of fusion, specific heat capacity, and cost, are considered to calculate its efficiency. In this research, PCMs were selected based not only on their efficiency and cost but also on their life cycle inventory data. This method is important because LCI data provide information about the amount of energy used, input and output from the system, emissions, and by-products from cradle-to-gate. Results and discussion have proven that mixtures of PCMs perform better than single-compound PCMs. Though the ternary compound costs three times the amount of sodium nitrate, its performance is 1.8 times that of sodium nitrate. In addition, results prove that nitrate-based single-compound PCMs are more efficient than other single-compound PCMs, and PCM mixtures with different melting temperatures perform better than single-compound PCMs. Using this approach for selecting PCMs is more efficient, economical, and eco-friendly. Regarding the environmental impact of building envelope applications by phase change materials, it is obvious that PCMs have made a noteworthy environmental impact compared to the majority of conventional construction materials. This impact differs based on the type of PCMs. Furthermore, considering the environmental impacts of the PCM utilized in heating and cooling systems, primary impacts can be reduced using PCMs along with an oil and gas system. Based on the findings of this research, it can be concluded that a life cycle inventory can be an important method to identify and assess the sustainability of phase change materials. As a future work, uncertainty analysis can be performed on some of the selected materials since it is an important analysis for the decision-making process for the PCM selection.

Abbreviations kWh, Kilowatt-hour; LCA, Life cycle assessment; LCI, Life cycle inventory; MJ, Megajoule; PCM, Phase change material; TES, Thermal energy storage

List of symbols τ, Density fraction; ρ_{bi}, Density of binary compound PCM; ρ_{A}, Density of compound A; ρ_{B}, Density of compound B; ρ, Density of PCMl; C_p, Specific heat capacity of PCM; λ_{bi}, Thermal conductivity of binary compound PCM; λ_{A}, Thermal conductivity of compound A; λ_{B}, Thermal conductivity of compound B; k, Thermal conductivity of PCM; e, Thermal effusivity of PCM; W_A, Weight of compound; W_B, Weight of compound B; ΔH_m, Heat of fusion

Table 6 Emissions data for PCMs

PCM No	Emissions to air	Emissions to water
C1: $NaNO_3$ (100.00)	Carbon dioxide = 0.5177 kg	Carbonate = 0.0372 kg Nitrate = 0.0384 kg Sodium ion = 0.0285 kg
C3: KOH (100)	Water = 0.0013 m^3	Chloride = 0.0380 kg Potassium ion = 0.0130 kg Water = 0.0031 m^3
C4: KCl (7.18) + KNO_3 (92.82)	Hydrogen chloride = 0.67×10^{-6} kg Particulates < 2.5 um = 0.553×10^{-7} kg Particulates > 10 um = 0.1×10^{-5} kg Water = 0.0004 m^3	Chloride = 0.009 kg Magnesium = 0.0009 kg Sodium ion = 0.0053 kg Sulfur = 0.0009 kg Calcium ion = 0.0002 kg Potassium ion = 0.0001 kg Water = 0.0007 m^3
C5: KNO_3 (65.31) + K_2CO_3 (34.69)	Carbon dioxide = 0.0058 kg Water = 0.0032 m^3	Hydroxide = 0.0045 kg Potassium ion = 0.1030 kg Water = 0.0051m^3
C7: Na_2CO_3 (56) + Li_2CO_3 (44)	Ammonia = 0.0011 kg Water = 0.0227 m^3	Calcium ion = 0.0560 kg Chloride = 0.1344 kg Nitrogen = 0.0001 kg Solid inorganics = 0.0556 kg Water = 0.0367 m^3
C8: KCl (54.75) + LiCl (45.25)	Particulates < 2.5 um = 4.2×10^{-7} kg Particulates > 10 um = 0.7665×10^{-5} kg Carbon dioxide = 0.2370 kg Hydrogen chloride = 0.0008 kg Water = 0.0077 m^3	Chloride = 0.0880 kg Magnesium = 0.0062 kg Sodium ion = 0.040 kg Sulfur = 0.0068 kg Carbonate = 0.0170 kg Lithium ion = 0.0040 kg Calcium ion = 0.0011 kg Potassium ion = 0.0009 kg Water = 0.0122 m^3 Total organic carbon = 0.0079 kg
C9: K_2CO_3 (22.05) + KOH (77.95)	Water = 0.0031 m^3 Carbon dioxide = 0.0037 kg	Chloride = 0.0296 kg Potassium ion = 0.0101 kg Water = 0.0057 m^3
C10: K_2SO_4 (16.54) + KOH (83.46)	Particulates < 2.5 um = 0.196×10^{-8} kg Particulates > 10 um = 0.62×10^{-8} kg Water = 0.0011 m^3	Chloride = 0.0317 kg Potassium ion = 0.0108 kg Water = 0.0026 m^3
C12: Na_2CO_3 (37) + K_2CO_3 (35) + Li_2CO_3 (28)	Ammonia = 0.0008 kg CO_2 = 0.0059 kg Nitrogen = 0.0067 kg Water = 0.0183 m^3	Calcium ion = 0.0390 kg Chloride = 0.094 kg Inorganic solids = 0.0367 kg Nitrogen = 0.0001 kg Hydroxide = 0.0045 kg Potassium ion = 0.0104 kg Water = 0.0291 m^3

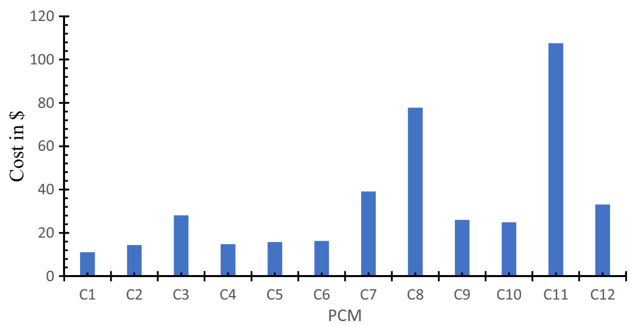


Fig. 6 Cost data for PCMs

Declarations

Conflict of interest The authors declare no competing interests.

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