



Expert Systems and Artificial Intelligence Importance in Using Phase Change Materials in Thermal Applications: A Review

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ABSTRACT

The accelerated development of energy requirements and climate change reduction brought about an increase in the study on novel thermal energy storage systems. With its latent heat capacity, Phase Change Materials (PCMs) have become a promising medium, as it is capable of absorbing and releasing large amounts of latent heat during the process of changing phase. This is a critical review of the involvement of expert systems and artificial intelligence (AI) in developing the selection, design, and use of PCMs in several thermal processes. The paper classifies PCMs into the following types; organic, inorganic, and eutectic and discusses their thermal characteristics, advantages and limitations. The issues that receive special consideration are the low thermal conductivity, supercooling, phase segregation and cost obstacle. The involvement of expert systems in PCM can be seen to support its deployment by replicating human experience, supporting material selection, and configuration of a system across different thermal and economic situations. At the same time, AI technologies such as machine learning, neural networks, and fuzzy logic allow predicting the behavior of PCM correctly, optimizing the working system in real-time, and managing uncertainty. Moreover, when combined with the use of nanotechnology and IoT, AI has also brought smart PCM systems that can predict maintenance services and apply adaptive thermal control. The paper uses this as its culmination at the end to indicate the future directions with respect to AI-assisted material discovery and superior hybrid PCM systems placing them as critical to the next-generation sustainable power solutions.

1. Introduction


The global energy consumption continues to increase, and the immediate demand to address the problem of climate change stresses the necessity to find optimal and environmentally friendly ways of energy storage. Phase change materials (PCMs) are part of the innovative choices as far as thermal energy storage is concerned.

Preferably, they can absorb and give off huge quantities of heat during phase changes contributing to maintenance of constant temperatures. This renders PCMs to be useful in areas such as renewable energy, building climatic regulation and cooling of electronics.

The PCMs can be used to store energy as only high and low states occur in solid and

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liquid phases, as described in Section 2.1. When they melt, they absorb heat belonging to their environment and as they solidify, they emit the same heat. This back and forwards provides a clever means of dealing with heat loads. Types of alloys are a range of organic, inorganic, and eutectic; it is possible to select one depending on the melting points and heat conduction.

PCMs have been used especially in solar energy systems. Conventional thermal storage is prone to failure owing to the slow promotion of heat transfer, or the appearance of the supercooling phenomenon, which have been mentioned in Sections 2.2 and 3.1. In response, the current development of PCM technology is directed at intelligent design nuances such as the enhancement of heat exchange surfaces and encapsulation. These inventions enhance productivity and reduce losses such as leaks, or breakages of materials.

In addition to material improvements, expert systems have become so significant in implementing PCMs as in 4.1 and 4.2. By extracting human experience in knowledge resources and logic programs, the systems are useful in the selection of the most suitable materials by balancing thermal characteristics against expenses. They also facilitate real-time tracking of data, which makes it possible to make adjustments that are fast responding to the changing environment.

Artificial intelligence also drives the further optimization of PCM that is emphasized in Sections 5.1 to 5.3. AI will then apply machine learning to consider previous temperature records and predict future thermal needs using machine learning. Neural networks and fuzzy logic techniques enhance the efficiency of PCM design, as well as the durability of the system in extremely different conditions.

Still, challenges remain. Section 3 and Section 7 note these barriers such as high

costs and incompatibility with existing infrastructure that should be addressed, despite the promise of AI integration.

Moving further to Section 8, current studies researches on AI-based capabilities that may produce innovative materials with a higher level of qualities or even versatile composites that can be used in various environments.

Overall, the introduction presents phase change materials as key contributors to thermal management, which can provide a sustainable solution to satisfy gradually increasing energy demands and deal with the reality of a changing climate, R & Rajagopal, 2024, [1], Hamzat et al., 2025 [2] and Diaconu et al., 2022 [3].

2. Overview of Phase Change Materials

2.1. Definition and Characteristics of PCMs

Phase Change materials (PCMs) are substances that retain and release energy by interchanging the state to become solid and liquid phases. They do not ferment, but now carry away the heat in melting, and then give it forth in solidifying. Such attributes as the thermal conductivity, melting point, operating temperature span, and energy storage capacity and the heat of fusion are major factors that influence the performance of a PCM.

The speed of PCM transfer of heat is dependent on thermal conductivity. High conducting materials are more effective in resisting temperatures. Normal organic PCMs have low conductivity, and slow down heat transfer and this is a barrier in their application in certain applications.

Melting point that of a PCM is the temperature at which it is in a change of phase. To be operational with the system, it is worth matching this point with system needs. When it fails to coincide, the PCM may run too often or it cannot perform at its best, which means that its life is short.

Energy storage capacity shows the amount of heat that is stored by PCM per unit mass. The larger the latent heat capacity, the higher the amount of energy that can be stored by the material with less temperature. This will render PCMs useful in heating and cooling systems where they will be of benefit in ensuring that there is constant temperatures to enhance comfort and efficiency.

Heat of fusion is used to measure latent heat taken or given out in the change of phase. When the values are larger, the PCM is capable of managing a greater amount of energy throughout the melt-solidification process/process, and this is advantageous to thermal management.

The pcm are classified into organic, inorganic and eutectic. Organic PCMs can be highly stable and contain large quantities of latent heat, but they are likely to be flammable, with low thermal conduction. Heat can be moved more effectively and more energy stored with inorganic PCMs such as salt hydrates or metals but this can undergo supercooling leading to unpredictable operation. The mixtures of PCM, eutectic, have lower type of melting than all its components, increasing the stability and control, and are applicable to HVAC and battery cooling.

Recently, nanotechnology has been used to enhance PCM thermal conductivity to enhance the efficiency and increase their area of use.

Learning these properties, it is possible to choose the appropriate PCM and create effective thermal systems in different industries, Mohammed et al., 2025 [4], Reddy et al., 2024 [5] and Awan et al., 2023 [6].

2.2. Classification of PCMs

2.2.1. Organic PCMs

The sources of organic phase change materials (PCM) are primarily of hydrocarbon origin and decompose into

two major groups that are the paraffins and fatty acids. The PCMs contained paraffins have vast applications in thermal applications due to their ability to retain a lot of heat thus being good in storing energy. They contain a huge capacity of latent heat and thus they can absorb and emit substantial thermal potential when melting and solidifying. This increases paraffins usefulness in cooling technologies particularly.

What is interesting about fatty acids is that they are environmentally friendly since they are biodegradable and can be replenished in the run of time. This contributes to their being appealing options in situations as far as environmental safety is concerned. They possess differing thermal behavior, and their melting temperatures depend on the length and structure of their carbon chains, which on their part influence this.

The good property of organic PCMs is that it is chemically stable at several heating and cooling cycles. This implies that they retain their performance in long durations with little wear, which is important when there is a need to seek durability in an application. In addition, those materials are more likely to be easier and less expensive to created than others do.

Nevertheless, there are such disadvantages of organic PCMs. A major concern is flammability as most of the organic substances may easily become fire able and hence, one should be careful in handling them and institute the appropriate safety measures. In addition to that, they usually possess good latent heat storage, but their thermal conductivity in solid form is subpar to inorganic PCMs. Such reduced speed of heat transfer may decrease the efficiency in the process of charging and releasing energy.

In the recent past, efforts have been made to increase these thermal properties by encapsulation or mixing with materials such as graphite or carbon nanotubes.

These modifications improve the ability of transfer of heat and retain great latent heat simultaneously.

Researchers to specific applications have also customized organic PCMs. Mild response With solar-thermal storage, another important factor is the ability to store and release energy by a quick phase change. In medical applications, their compatibility with biological systems has provided an opportunity of temperature sensitive drug delivery, where accurate

control of heat is the key to an effective treatment.

Overall, organic PCMs can be viewed as a versatile technology that can be applied in every field of life, including clean energy and medicine. As further developments are made, it is expected that the future of less toxic, more effective organic phase change materials will be positive as it expands its avenues in various industries, Goel et al., 2023 [7], Zare & Mikkonen, 2023 [8] and Cartagenas, 2025 [9].



Figure 1: Sample of paraffin wax, Cartagenas, 2025 [9].

2.2.2. Inorganic PCMs

Inorganic phase change material (PCM) which is mostly composed of salt hydrates and metals implement a range of benefits to thermal management. These inorganic are generally more thermal conductive and higher energy density than organic PCMs and can be packed with a higher energy density. They are therefore suitable in application where high heat transfer and large energy storage is required. Sodium acetate trihydrate were interesting salt hydrates since they are effective in the moderate temperature, commonly between 8 degrees Celsius and 120 degrees Celsius. The materials are the one you will use in the construction of temperature control,

solar water heater and up to temperature-controlling textiles.

The ability of inorganic PCMs to store a lot of heat, the little amount of volume that it undergoes during transitions, low cost and non-existence of fire catching make inorganic PCMs shine. They absorb heat significantly as well as maintain temperatures unchanged through changes of phase- that is ideal where consistent thermal performance is of importance.

With this, inorganic PCMs have certain challenges. It is a challenge to do supercooling, in which the material does not solidify at the desired temperature. These materials are susceptible to corrosion and other inorganic salts can lie apart as time goes and this is detrimental

to their performance. In addition, some PCMs that use metals can be quite expensive as compared to those that use organics.

Researchers are addressing these concerns by incorporating nanomaterials in inorganic PCMs what is termed to be nano-enhanced phase change materials (NEPCMs). The technique enhances thermal conductivity, in others; addition of carbon nanoparticles can give up to 25. This is because such improvements enhance rapid heat flow through systems that have these improved materials.

New uses are also made available by inorganic PCMs. They are catching up on concentrated solar power plants since they

can tolerate high temperatures and store superabundant heat produced at the day of the peak sunshine. Similarly, they are also applied in extraction of industrial waste heat where heat management is of great importance.

In conclusion, the inorganic PCMs hold a good future path to the enhancement of energy storage due to the high latent heat and due to the enhanced heat transfer with the aid of nanotech. Nevertheless, such issues as supercooling and chemical wear still need more efforts and inventions to make these materials even more dependable and helpful, Cartagenas, 2025 [9], Varol et al., 2010 [10] and Liu et al., 2023 [11].

Table 1: Summary of the abbreviations used for PCMs, supporting materials, and additives, Liu et al., 2023 [11].

Classification	Material		Abbreviation
Phase change materials	Organic materials	Polyethylene glycol	PEG
		Paraffin wax	PW
		Lauric acid	LA
		Stearic acid	SA
	Inorganic materials	Vanadium dioxide	VO ₂
Supporting materials	Organic materials	Polystyrene	PS
		Polyvinylpyrrolidone	PVP
		Polyvinyl alcohol	PVA
		Polyacrylonitrile	PAN
		Cellulose nanocrystals	CNC
		Polymer-polymethyl methacrylate	PMMA
		Melamine-formaldehyde	MF
	Inorganic materials	Graphene oxide	GO
		Boron nitride	BN
		Carbon quantum dots	CQDs
Carbon nanotubes		CNTs	
Other additives	Organic materials	Imipenem	IMP
		Doxorubicin hydrochloride	DOX
		Polydopamine	PDA
	Inorganic materials	Zeolitic imidazolate framework-8	ZIF-8
		Black phosphorus	BP

2.2.3. Eutectic PCMs

Eutectic phase change materials (PCMs) unique feature is the sharp melting (solidification) at one single temperature, below that of each of the individual components. This occurs when they are mixed to comprise eutectic mix of two or more PCMs. It is due to this that eutectic systems have lower melting point than regular PCMs thus increase their thermal efficiency and energy storage.

Such eutectic PCMs are organic and inorganic. Organic eutectics normally combine fatty acids or paraffin wax and inorganic eutectics are the ones that combine metal salts or salt hydrates. This mix and match aspect allows designers to adjust properties of a given mix such as melting temperature and latent heat to suit various requirements.

Eutectic PCMs have a dense energy storage that is one significant advantage of this type of PCMs. Being able to change phases in a small temperature possession, they are capable of absorbing and giving up huge volumes of heat with minimal temperature change. This makes them an ideal option in any thermal system that needs narrow temperature regulation like HVAC systems in a building, or coolers in a battery.

Individuals have begun to impregnate building materials with encapsulated eutectic PCMs in construction. This reduces thermal mass and ironing out of temperature variation and helps reduce energy required to heat and cool buildings. Indicatively, the addition of eutectic PCMs into cement does not only enhance the cement but also thermal stability and generated latent heat to maintain the comfortable conditions in the interiors.

In selecting the appropriate eutectic PCM, one will have to compromise against criteria such as its compatibility with other building materials, cost and its sustainability in terms of survivability in a

large number of cooling and heating cycles. Conducting thermal cycling tests is a way of ensuring that the PCM retains its properties during the useful life of its existence.

Scientists are busy ensuring that eutectic PCMs can be further improved. They are trying composites and other advanced techniques of encapsulations in order to accelerate heat transfer and prevent leakage in the liquid state.

Overall, eutectic PCMs are a versatile set of tools to manage the thermal energy in any industry/construction industry to renewable energy. Their combination of various qualities into a single substance gives them new possibilities of storing and transferring heat in the most types of systems, Reddy et al., 2024 [5], Podara et al., 2021 [12] and Togun et al., 2025 [13].

3. Challenges in PCM-Based Thermal Systems

3.1. Material Limitations

PCMs are important in the thermal energy storage where the substance takes up and gives out the heat during the phase change. However, a number of material disadvantages restrict their popularization and diminish their effectiveness.

One of the challenge hurdles is due to the low thermal conductivity predominant in most PCMs. This causes slowness in heat transfer due to phase changing which results to slow heating or cooling. This slow reaction can result in increased time operations of the PCM based systems to achieve intended temperatures thereby leading to the increase of the energy consumption. As an illustration, most typical organic and inorganic PCMs hardly provide adequate conductivity to enable rapid heat exchange that requires a longer run time and higher expenses.

There is also supercooling as a problem. Other PCMs remain liquid at lower temperatures than freezing point without

solidification and their ability to emanate heat is erratic. The PCM is not able to provide the latent heat projected in time when solidification does not take place.

This compromises a robust energy storage and makes control mechanisms difficult.

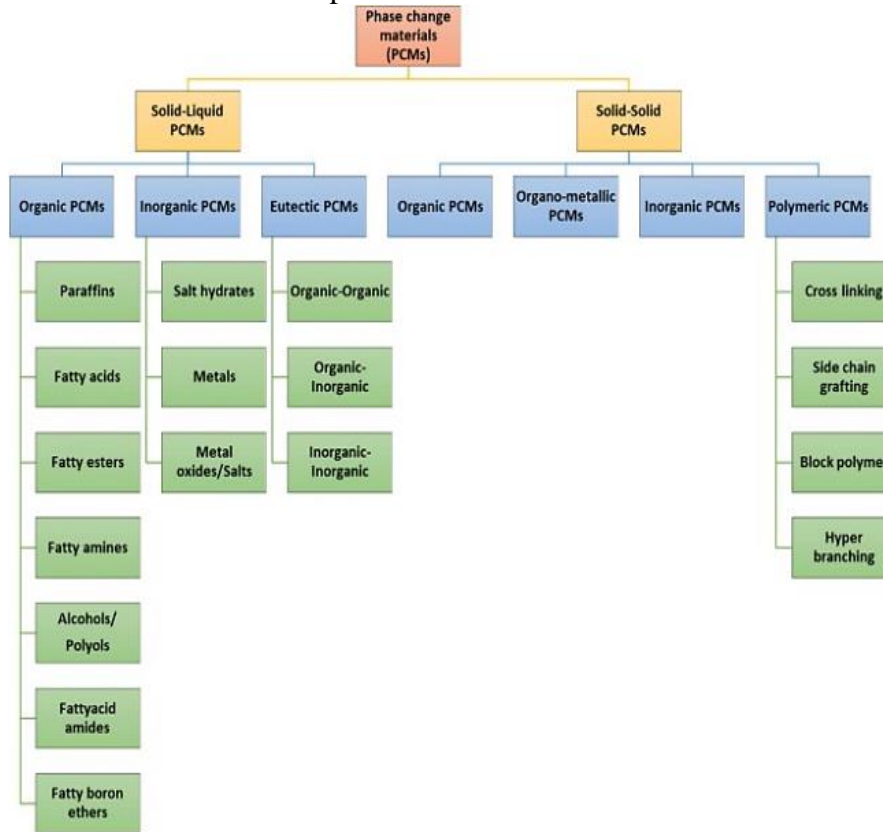


Figure 2: The broad classification(up-to-date) of the phase change materials based on their phase change behavior and composition, Reddy et al., 2024 [5].

The changes in volume PCM goes through when melting and solidifying further complicate it. Both expansion and contraction may cause mechanical friction damaging to the containment structures or jeopardizing the stability of the system even in cyclic conditions. Moreover, there are PCMs that have the problem of phase segregation, whereby the components are segmented when they are used and deteriorate over time.

Encapsulation also poses some challenges. Good encapsulation should not have leakages and should enhance thermal conductivity by making intelligent decisions on shell materials and shapes. Unstructurally designed shells can either fail or lower the efficiency of heat transfer by prohibiting contact between PCM and environment.

In an effort to address certain shortcomings, composite PCMs, that incorporate pure PCMs and conductive additives, such as metal foam or nanoparticles. Although they enhance better heat conductivity, these composites introduce new challenges on manufacturing and cost efficiency. It is difficult to assure even distribution of the additives to the disadvantage of the underlying properties of PCM.

Nanotechnology points to good breakthroughs to improve PCMs more, by nano-enhanced composites or by nano-scale confinement. Nevertheless, the innovations are challenging to scale up in a cost-effective manner. The implementation of such advanced materials into practice requires high costs in research, and an understanding of their impacts on the

lifecycle, both economically and in regard to environmental factors.

It is crucial to overcome these obstacles by some ingenious engineering to realize fully the potential of PCM in a multifarious variety of thermal management

applications, as construction material or state-of-the-art in battery cooling, Goel et al., 2023 [7], Togun et al., 2025 [13], Alagumalai & Mahian, 2022 [14], Aftab et al., 2018 [15] and Radouane, 2022 [16].



Figure 3: Graphical abstract: Nanoconfined phase change materials for thermal energy applications, Aftab et al., 2018 [15].

3.2. System Design Issues

A system based on Phase Change Materials (PCM) has a number of challenges that have to be overcome in order to increase its efficiency and viability. Selecting the appropriate PCM is one of the primary problems, which necessitates the balancing of such aspects as the melting point, thermal conductivity, and compatibility of PCM and encapsulation materials. Largely, the success of the PCM depends on its thermal properties; if the thermal conductivity is low, heat transfer is slow, and therefore, great design tricks are required to resolve this bottleneck.

Another important factor will be the physical design of the PCM in the storage arrangement. The layout of the PCM layers, and the thickness of both, can have a significant impact on the performance of

the systems. Poor heat flow and increased phases change times tend to be caused by uneven distribution. It implies that designers need to be attentive to the homogeneous distribution and use the maximum thicknesses possible in order to achieve the optimum amount of heat transfer.

Encapsulation also acquires a very significant part. Selecting the appropriate shell materials ensures that the PCM is not destroyed, and it assists in taking out the heat effectively between the PCM and the surrounding environment. The form and design of such shells must be able to expose as much surface to contact as possible and minimize thermal resistance. It has been demonstrated that by means of porous foams, or prolonged surface areas, conductivity can be greatly enhanced and surpass the capability of traditional shells.

There is a problem with long-term durability. Associated with many PCMs can shorten or lengthen by up to 20 percent when melting or solidifying; thus, encapsulation or other components need to be considering this effect. In addition, the repeated heating and cooling can lead to degradation or change of characteristics of some PCMs, which is relevant to the level of reliability of the system in the long term.

Bringing PCMs into the current technologies is in itself a challenge. The use of applications such as battery cooling of electric cars or saving power in buildings would require specific solutions because of varying conditions of work. Such diversity renders solutions to universal answers challenging to use.

Design decisions also have a heavy weight due to economic reasons. Having highly specialized systems in each application may be prohibitively expensive and therefore the need to tradeoff between standardization and flexibility may be a solution to its distribution without crippling the bank account.

Finally, it is essential to do extensive testing in working conditions. Assessment of the models using real-world data is crucial to making sure that systems perform according to the specifications and to enable the developer to make constant improvements in designs. Setting up explicit performance standards will assist in terms of comparison of various PCM systems and driving continuous changes, Diaconu et al., 2022 [3], Goel et al., 2023 [7], Jinhua Chi, 2023 [17], Sevault, 2018 [18] and Ismail et al., 2022 [19].

3.3. Cost Considerations

The application of Phase Change Materials (PCM) in thermal systems poses great costs that influence their wider application and performance. The first problem is the

cost of PCM-based arrangements in the first place. The improved technology and the use of advanced materials in products frequently result in a higher cost of the high-performance PCMs compared to traditional thermal storage products. This initial cost may be an obstacle particularly to the smaller companies or projects with low budgets.

In addition to the material price, there is also the operating cost. Costs can go high with installation, maintenance, and the process of implementing PCMs into the current systems. The process of developing effective PCM is usually complicated resulting in increased engineering and design costs. There may also arise additional costs associated with research and optimization since a significant portion of PCM technologies is still in its development, and this factor is likely to make the overall prices even more unpredictable.

The economic research has given varied outcomes on the benefits of PCM adoption in savings basing on the usage. An example here would be the introduction of PCMs in green houses to reduce power consumption and reduce carbon emission. These advantages, however, depend on such factors as location and type of PCM. Although it may seem that the operational savings including decreased energy bills may become visible in the early stages, the initial investment will be more recouped than expected in the long run since the initial cost in the industry is quite high.

Lifecycle costs introduce some added dimension on the picture. When sourcing and processing of PCM materials is linked to an environmental impact, the financial implications may arise, particularly in cases when the environmental regulations or other incentives related to sustainability are introduced. The companies must not only consider material cost but also the long-term cost that may occur in terms of compliance costs associated with the environment.

Budgeting is also complicated by the fluctuations in supply chain. Raw materials prices in PCM formulas are unpredictable due to changes in the market, where it becomes difficult to negotiate constant costs of the projects.

Pricing is also affected by the rivalry in the market. With the entrance of a larger number of producers cheaper or better performing PCM products, prices can eventually go down. Nevertheless, eventually, the cost will be a major impediment to a broader application until the innovations become widespread or are manufactured on a larger scale.

Moreover, more specialized system designs, in order to match PCMs, should provide a way to circumvent certain material constraints, although such more specialized configurations require additional initial investment. This trade off must be studied carefully to show whether the future returns will be worth the initial cost.

Ultimately, the resolution of these cost-based problems requires consideration of both material choices and approaches to implementation. It will be critical that PCMs are able to balance the economic reality and the individual needs of thermal energy storage systems so that they can achieve their full potential, Diaconu et al., 2022 [3], Reddy et al., 2024 [5] and Alagumalai & Mahian, 2022 [14].

4. Role of Expert Systems in PCM Applications

4.1. Definition and Functionality of Expert Systems

Expert systems form part of the artificial intelligence that is meant to imitate the decision-making processes of human experts. They depend on a set of rules and knowledge in order to address complex issues, particularly those that encompass specialized knowledge. Such systems include two major components: knowledge

base that contains facts and other types of heuristics about the topic, and an inference engine that can be utilized to arrive at conclusions based in the information stored about it using logical rules.

In the context of phase change materials (PCMs) and their applicability in thermal systems, in general, expert systems may come in quite handy to tune the examples of materials and systems, as well. Such AI tools evaluate different aspects such as thermal characteristics, cost-efficiency, and environmental impact of alternative PCMs. As an illustration, organic and inorganic PCMs are different in their characteristics such that they are applicable to some applications, as explained above. The expert systems assist the engineer to identify the most appropriate materials based on the anticipated conditions of operation.

Their worth transcends beyond the provision of recommendations. Through connection of sensors to expert systems, real-time analysis on temperature variation, phase transformation and heat storage may be done continuously. This continuous analysis makes this a feedback loop, which can be treated by adaptive control to enhance system performance by adapting to changing conditions based on energy requirements.

In addition, as noted in previous portions of this paper on challenges associated with system design, expert systems may be used to experiment with various technical configuration choices that may be made on incorporating PCMs in thermal systems. The initial process of their inference engine replicates the behavior of the system in different circumstances and this reduces the trial and error that normally accompanies the engineering designs.

Such systems are luminous when they address the uncertainty that is bound to be present in Xbox behavior when changing between phases which are studied in the context of application of fuzzy logic.

Experimental systems are used to make decisions in the face of unpredictable influences such as temperature fluctuations in the atmosphere or material abrasion with time by coding rules using historical information and experience.

Besides, the use of expert systems can enable companies to fasten training of engineers or technicians who, perhaps, have no profound experience of PCM technology. Teams will be able to keep the quality on the right track with more efficiency because centralized knowledge will give them clear and step by step instructions based on the best practices and the lessons that were learnt somewhere before.

Simply put, expert systems are important in the PCM applications in case of assisting well-informed decisions that were made based on a large amount of special knowledge. Concurrently, they allow systems to adapt to conditions that are presented in the real-life, both in implementation and in working, R & Rajagopal, 2024 [1].

4.2. Expert System Frameworks for PCM Analysis

Expert systems are used to complement the thermal management of phase change materials (PCMs) to include expert knowledge and decision-making instruments. They ease the process of selecting the right kind of material and optimization of designs. These systems consider thermal characteristics and cost efficiency, which is significant because of the complicated nature of the phase changes and performance influence.

Expert systems use simulations to determine the response of the various PCMs to the varying conditions. This assists designers to adopt superior thermal managerial options. Assuming they are connected with real-time monitoring, they are able to reuse control strategies in real-

time to ensure maximum efficiency. They may also be used as examples by following up on environmental developments and previous data to manage stored energy in PCMs. This is very handy in the solar thermal energy storage and residential climate regulation where the conditions are not invariably the same.

The use of PCM has uncertainties that the expert systems deal with. Instead, they simulate a variety of designs to deal with such challenges as volume changes in case of phase shifts that may lead to structural inconveniences. This assists in identifying solutions that minimize a risk of materials.

These systems are enhanced through the incorporation of artificial intelligence that allows the ability to continually learn new information. Machine learning enhances the future predictions of PCM behavior based on the present and the past; hence at some point decisions are more precise.

The various frameworks offer different approaches. Others allow users to be able to enter in specifications like the melting point or heat transfer requirements to obtain certain material suggestions. Others provide platforms to have the visualization of the thermal system interactions, and help to explore the different variables.

The introduction of the IoT technology provides real-time information of sensors in applications. This real-time information enhances decision making because it shows PCM performance at any given time.

Still, in a word, the expert system is not merely an analysis; it is a driver of the PCM application innovation. They optimally use energy in the buildings and give accurate thermal control in the industries. With automated intelligence and interfaces, new opportunities will arise in the potential applications of PCM since such technologies will be more accessible and effective, R & Rajagopal, 2024 [1] and Zhang & Strbac, 2025 [20].

5. Applications of Artificial Intelligence in PCM Optimization

5.1. Machine Learning Techniques for PCM Performance Enhancement

This new technology of machine learning (ML) has proved to be the friend of augmenting the performance of phase change materials (PCMs) in a variety of thermal apparatus. With the exploitation of large volumes of data and advanced algorithms, ML can be used to refine PCM properties in order to achieve enhanced energy storage, temperature regulation, etc.

The main aspect of optimization of PCMs is the prediction of the key thermal parameters such as latent heat, thermal conductivity, melting points and the rates of heat transfer. The machine learning models are capable of browsing historical data predicting the behavior of PCMs in various situations. As an example, regression procedures are used to estimate latent heat capacity or conductivity using previous experiments. These discoveries help researchers to shortlist the potential PCMs even before they are observed experimentally.

In addition to the prediction of properties, the ML algorithms are used to achieve the best PCM formulations. Genetic Algorithms and Artificial Neural Networks are tools that are tested on a variety of material combinations within relatively a short period, taking into account such factors as cost, environmental effects and stability during temperature fluctuations. This methodology reduces the volumes of data available in earlier research literature that are useful in identifying PCMs appropriate to specific applications with more speed and accuracy.

Moreover, ML is a good aptitude to simulate the PCM behavior real-time when changing phases. The AI-based digital twins of thermal setups can offer

continuous simulations that would assist in controlling the system performance under varying thermal loads. This real-time knowledge directs the decisions when to absorb or warm up heat and this improves the management of energy.

One of the most promising sectors is the learning of machine learning and the IoT technology. Thermal systems are fitted with smart sensors that directly record live information about the change in temperature and power consumption associated with PCMs. The input of this data into ML models reveals patterns and allows the optimization of system controls uninvolved, which will lessen the necessity to manually adjust them.

Machine learning is also important in determining the influence of additives on the performance of PCM. Thermal conductivity is also increased with addition of nanoparticles or expanded graphite, however, locating the optimal mix and distribution would require sophisticated modeling in ML. These algorithms calculate the performance of various additives on the systems based on predictive simulations.

Ultimately, machine learning provides incessant optimization, at not only the PCM selection and design but also the response to new operation data. This continuous learning cycle contributes to the creation of smarter and more responsive PCM ways of solving that would address the current needs and be able to foresee the future challenges in thermal management, R & Rajagopal, 2024 [1].

5.2. Neural Networks in PCM Modeling and Prediction

Neural networks have been a desirable resource in the modeling and prediction of phase change materials (PCMs). Their advantage is in identifying complex trends of great datasets when it comes to the

nonlinearity of PCM thermal dynamics in numerous conditions. These networks can be used to predict important thermal characteristics using previous information and predict the, melting and solidification temperatures, heat storage, and response times, reliably and efficiently.

The uniqueness of the neural networks is the possibility to deal with various input factors such as material properties, environmental effects or system configurations. Such flexibility gives scientists the ability to design forecast models that meet specific purposes, be it in enhancing energy storage systems or in enhancing buildings thermal performance. The type of data and the accuracy of prediction required due to the type of data typically defines the different types of neural network structures that are selected such as feedforward networks, recurrent neural networks (RNNs), and convolutional neural networks (CNNs).

The general steps to apply neural networks in PCM studies include using the dataset to prepare the study, training the model, validating its performance, and lastly deploying the model. The dataset should also have a diversification of operating situations in a way that the model works at the board level. The processes during training use algorithms like the backpropagation to adjust the weights of the network and achieve the optimum predictive power. Validation checks the way the model will make use of new data and avoid overfitting, which ensures reliability in post-training usage.

It is also possible to improve the modeling performance with the use of neural networks in addition to other optimization techniques. As an example, adding physics-based constraints can be used to construct easier-to-interpret models, which also use the advantages of deep learning. In addition, neural networks can also be used as a substitute of complex simulations or fluid dynamics

computations frequently needed during PCM analysis.

These advanced models are used in variety of PCM applications such as in renewable energy storage systems and in thermal storage in buildings and industrial processes. The ability of neural networks to handle real-time data is also being used to create adaptive control systems that adjust the performance under the changing external conditions to increase overall efficiency.

With the development of the field, scientists are looking to make these models better explain their findings; adopt newer models such as explainable artificial intelligence (XAI). These enhancements are not only in order to add more edge when it comes to forecasting but also create more confidence within the engineers as well as the stakeholders who use these brilliant tools to make crucial decisions that involve phase change materials, Isania & Galgaro, 2025 [21], Zhang & Strbac, 2025 [8] and Mohammed et al. [22].

5.3. Fuzzy Logic for Uncertainty Management in PCM Systems

Fuzzy logic is tremendously important in dealing with the ambiguities that are prevalent in the operations of phase change material (PCM). Thermal behavior of PCMs is sensitive to numerous factors, such as variation in ambient temperature, change in heat load, variation in the material properties that may change either with time, or with phase transitions. In such situations where unexpected factors arise, traditional control methods tend to fail. Fuzzy logic, however, provides a more adaptable approach to process of working with vague or incomplete information that is a close resemblance to real life.

In its core, fuzzy logic emulates human reasoning due to its capability to address

the different levels of truth rather than aim to employ a rigid system of true-or-false. This ability comes in particularly useful during the use of PCM where the accuracy of the pins would be difficult to obtain due to changes in the environment. Considering the example of thermal management, it is more flexible since fuzzy logic may operate under a range of temperatures rather than having the exact values.

PCM systems duplicating the gone are fuzzy logic controllers: in real time, they can adjust operating parameters using real time data. They are based on the membership functions that take the input variables (like temperature or energy requirements) and convert them into a set of categories (like low, medium or high). The system is able to make decisions by the strength with which the inputs fall into these categories to determine when to store or exempt the heat. This plasticity would be useful in optimizing performance by varying PCM activity in response to the prevailing environment.

Fuzzy logic is applied in a variety of industries where PCMs are applied. Fuzzy controllers are used in the climate control of buildings to use indoors and outdoors temperatures mitigate heat accumulation and to control the flow of heat. Similarly, during the renewable energy systems such as the solar power systems, the variable nature of energy provision requires a control system that is fast acting and efficient. Fuzzy logic is very good at harmonizing current circumstances with the historic trend in order to ensure a smooth flow.

With machine learning, fuzzy logic and machine learning combine to increase its possibilities. In such hybrid models, control policies constitute a part of the continual improvement of these models, having learned to behave based on past system behavior. They become more predictive of any environmental changes or demand, but keep PCM efficiency.

The flexibility of fuzzy logic also contributes to the need to overcome certain obstacles associated with PCM properties such as the slow heat transfer of certain material. By considering these factors, adaptive controls are able to utilize available resources in the most effective way to increase the total reliability and performance of the systems.

Overall, fuzzy logic would provide an intelligent approach to dealing with the uncertainties related to PCMs. It allows making refined decisions by working comfortably with inexact data to achieve the same results regardless of the conditions, which is a major ingredient of efficacious thermal management in the current energy systems with phase change materials, R & Rajagopal, 2024 [1], Mohammed et al., 2025 [4], Zhang & Strbac, 2025 [20] and Mohammed et al., 2025, [22].

6. Integration of AI and Expert Systems in PCM-Based Designs

The combination of artificial intelligence (AI) and expert system with phase change materials (PCMs) changes thermal management to become more efficient, flexible, and accurate. AI is good at processing real-time and ensuring that the performance of PCM is maximized and forecasting the behavior of materials in various conditions. The result is development of superior designs in other sectors such as construction of climate control and electronic cooling.

The value addition of the expert systems is to replicate human reasoning to select appropriate PCMs. They also evaluate thermal characteristics including melting points and latent heat making sure that there is enhanced heat transfer and eliminating issues like supercooling and leakages. These systems, combined with AI, contribute to the more intelligent design decisions based on the conditions.

The adaptive learning of AI allows PCM systems to modify themselves on their

own accord with new information. They are also interconnected with the Internet of Things (IoT) and constantly oversee the material position and adjustment of thermal parameters. Indicatively, the

system is capable of augmenting the amount of heat it absorbs or releases anytime the cooling requirement increases and ends up performing optimally.



Figure 4: Diagram showing how AI techniques are being used in the thermal energy storage, Mohammed et al., 2025 [4].

Maintenance can also be improved through this combination in order to anticipate failure and address the problem beforehand. The position of PCM-based systems allows operators to design a repair or upgrade process that optimally extends the systems, adding to their longevity. In addition, the AI can assist in material innovation and modeling through simulation of new PCM formulations to help save the time and cost that is spent on the physical tests.

These advantages notwithstanding, there is still a challenge. It is imperative that the data should remain at its best level and efficient communication among various technologies demands effective protocols. Such measures will enable smooth functionality in the world of smart buildings to an optimum capacity.

Overall, the combination of AI and expert systems and PCMs will bring the thermal management to a new stage in numerous areas, including construction and renewable energy. This will allow making more intelligent decisions and will give a way to

new possibilities of efficient thermal control by combining progressive data analysis with the experience of experts, R & Rajagopal, 2024 [1], Reddy et al., 2024 [5].

7. Benefits and Limitations of AI and Expert Systems in PCM Use

The introduction of artificial intelligence (AI), as well as expert systems into phase change material (PCM), has a number of benefits and a number of constraints that influence its level of thermal management. Some of the advantages include enhanced efficiency concerning the use of PCMs through AI and expert systems. As mentioned above, the expertise systems are used to mimic the human experience to deal with complicated scenarios with numerous variables such as thermal characteristics and system pricing. The skill is useful in the selection of the best materials, as this is crucial because the appropriate thermal characteristics have a significant influence on PCM performance.

AI also assists in real-time monitoring and someone suggests controls that allow systems to respond rapidly to the changing circumstances in the environment. At the scale of big data, machine-learning algorithms can be used to identify trends that can inform more intelligent choices on the use of PCMs in energy storage. Such dynamism enhances a better use of energy and resiliency of the system because the status of live information optimally tweaks the amount of heat stored or released.

One more huge advantage is the fact that AI can facilitate predictive maintenance. Through monitoring the PCM work over a period the AI systems can predict when repairs, or replacement is required. Such proactive measure will assist in avoiding failures before they occur, and this is very critical in handling uncertainties as are common within PCM set-ups.

Although these advantages are present, there are certain shortcomings of implementing AI and expert systems in PCM. The first challenge is data dependency; AI models require many popular and high quality data to train. In the absence of that, the predictions might fail to hit the target, which would result in worse outcomes.

Implementation of AI in the existing thermal energy installations has interoperability challenges as well. These intelligent technologies should be able to interoperate with the current systems such as HVAC systems or energy storage systems and hence the designers must put into consideration the manner in which the various components will have to relate to each other.

Another factor is cost since the implementation of AI-solutions of PCM might involve large initial investment. This cost means that small organizations will not embrace the technology.

The expert systems can present a valuable contribution regarding the rise in scale with the help of simulations, but in some cases,

they cannot be scaled to a large number of climates, building codes, or applications. Geographical variations may make it complicated to roll out smoothly.

Lastly, questions of morality are raised because the application of AI-based devices in the context of decision-making in the field of thermal management becomes more significant. Liability of errors caused by autonomous AI systems is also an issue, as it is important to state that comprehensive testing and validation are needed in the first place, to avoid widespread implementation.

To the point, although the combination of AI and expert systems helps enhance PCM by a considerable margin, introducing such functions as predictive analytics and responsive control, it is important to acknowledge their data requirements, expenses, and integrability challenges, maximum scaling, and ethical aspects to use them successfully, R & Rajagopal, 2024 [1], Mohammed et al. [4] and Mohammed et al., 2025 [22].

8. Future Research Directions in AI-Driven PCM Discovery and Synthesis

The outlook of phase change materials (PCMs) research is very optimistic, and artificial intelligence (AI) is the driver of various exciting developments. A potential path to take is to create advanced machine learning models that will forecast and optimize the management of heat by current and future PCMs. A set of experimental and simulation data produces a large set of data that these algorithms search through and identify trends and nuances of relationship that would otherwise remain unnoticed. By manipulating PCM formulations, using such techniques as genetic algorithms, the researchers are able to achieve thermal performance enhancement and enhance the use of the available energy resources.

Composite phase change materials (cPCM) also provide many opportunities. Scientists can enhance thermal conductivity greatly by the addition of nanomaterials or highly conductive additives. The optimization tools using AI have the potential to provide an approach to scaling the interrelationship between mechanical, thermal, and chemical properties simultaneously to create PCMs with more tailored properties. With this flexibility, PCMs will be more suitable in addressing many requirements, such as energy management in buildings and storage of heat in renewable energy systems.

PCM manufacturing was another area that can be transformed by AI. Models of machine learning could automatize production by proposing the most efficient synthesis techniques, maximization of production, and reduction of the cost. The reinforcement learning provides an opportunity to explore new combinations or recipes of materials or devise better-performing ones faster accelerating the innovation process in the area.

The predictive maintenance based on AI, along with real-time monitoring, will make the PCM systems more dependable. The constant analysis of sensor data allows identifying possible problems before they occur, and AI models can perform fixes before a heavy malfunction occurs. This skill works well particularly, where it is necessary to protect sensitive data such as medical storage or cooling sensitive electronics where temperature is important.

Nanotechnology and AI together do not limit the PCM development even further. The nano-enhanced materials are not only working to enhance the material heat management, but also contribute towards ensuring sustainability through reduced reduction in material utilization during the manufacturing procedure. The future work should be focused on developing cost-effective and environmentally friendly PCMs and perfecting AI-based tools that

can serve in the multifaceted energy arrangements of these innovative materials.

The ability to scale up PCM applications to various temperatures and applications is still not an easy task. Designing of modular systems that would suit a range of settings without sacrificing efficiency or effectiveness could involve the assistance of AI and make it easier to broaden the adoption.

Lastly, it will need the cooperation of chemists, material scientists, computer experts, and engineers to advance AI-powered innovations in PCM. Promoting interdisciplinary cooperation and harnessing the power of potent computational tools such as deep learning in the context of thermophysical systems will create new opportunities in the solutions of heat storage that are more intelligent and efficient, Mohammed et al., 2025 [4], Radouane, 2022 [16], Zhang & Strbac, 2025 [20], Nemš et al., 2025 [23], Karyappa, 2025 [24] and Antolini et al., 2025 [25].

9. Conclusion

Phase change materials (PCMs) are evolving fast because of development in materials science. Since they are capable of absorbing and releasing heat when changing phases, they are applicable in energy storage, regulating the climate in a building, and in the temperature regulation of batteries. Their main characteristic such as a high latent heat and variable melting points make them useful in practice.

These PCMs are of three major categories namely organic, inorganic and eutectic PCMs that have different variations. Organic PCMs are environmentally friendly and are chemically stable although there are challenges on low thermal conductivity and flammability. Inorganic PCMs are more thermal conductive and have higher energy density, but are susceptible to supercooling and hence

unreliable. To balance between advantages and weaknesses, eutectic PCMs are made to combine the properties of both.

As it has its advantages, PCMs have challenges, which restrict their wider implementation. Low thermal conductivity reduces heat transfer and systems must be designed well to maximize the performance of the system. PCMs can be found in high initial costs that put off some users, although in the end they can save money.

Incorporation of expert systems is another method of enhancing PCM applications through historical data analysis with regard to the current conditions to determine the situation at a particular moment. Such systems are suggested to take the best arrangements according to material and operating parameters, which eliminates unpredictability of performance. Artificial intelligence also plays another role in PCM design to forecast thermal behavior as well as refine formulations with machine learning. Artificial Intelligence creates tailored software to store and provide power to industries and other renewable energy sources.

The fuzzy logic is applicable to overcome the uncertainty in the application of PCM, and thus to make decisions flexible with varying circumstances. This enhances resilience capabilities in the system in addition to addressing slow heat transfer.

Further investigation into AI-assisted discovery of new PCM formulations and advances using nanotechnology or hybrid materials such as liquid crystals can be performed in the future. High-end computational capabilities will facilitate the scaling process, as well as stability of materials in the end.

AI integrated with expert systems will be more efficient and cost effective in PCM technology coupled with accountability in smart systems. The sustained academia and industry work is critical in an attempt to ensure that present obstacles are eliminated to harness PCM potential in various

sectors. These innovations assist in an effort of achieving sustainable energy across the globe, as they help increase temperature control in buildings, battery cooling, among others.

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