

ТОРАЙҒЫРОВ УНИВЕРСИТЕТІНІҢ
ҒЫЛЫМИ ЖУРНАЛЫ

НАУЧНЫЙ ЖУРНАЛ
ТОРАЙҒЫРОВ УНИВЕРСИТЕТА

**ҚАЗАҚСТАН ҒЫЛЫМЫ
МЕН ТЕХНИКАСЫ**

2001 ЖЫЛДАН БАСТАП ШЫҒАДЫ



**НАУКА И ТЕХНИКА
КАЗАХСТАНА**

ИЗДАЕТСЯ С 2001 ГОДА

ISSN 2788-8770

№ 4 (2023)

ПАВЛОДАР

**НАУЧНЫЙ ЖУРНАЛ
ТОРАЙГЫРОВ УНИВЕРСИТЕТ**
выходит 1 раз в квартал

СВИДЕТЕЛЬСТВО

о постановке на переучет периодического печатного издания,
информационного агентства и сетевого издания
№ KZ51VPY00036165

выдано

Министерством информации и общественного развития
Республики Казахстан

Тематическая направленность

Публикация научных исследований по широкому спектру проблем
в области металлургии, машиностроения, транспорта, строительства,
химической и нефтегазовой инженерии, производства продуктов питания

Подписной индекс – 76129

<https://doi.org/10.48081/PWGH3542>

Импакт-фактор РИНЦ – 0,210

Импакт-фактор КазБЦ – 0,406

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МРНТИ 73.31.09

<https://doi.org/10.48081/NOWD5861>***V. S. Yessaulkov¹, K. Mahkamov²**¹Toraighyrov University, Republic of Kazakhstan, Pavlodar;²Northumbria University, Newcastle-upon-Tyne, United Kingdom*e-mail: yessaulkov.val@gmail.com**PONDERING THE CHOICE OF PCM AND MATHEMATICAL MODEL IN AUTOMOTIVE LHTS**

Phase change materials are latent heat storage materials. As the source temperature rises, the chemical bonds within the PCM break up as the material changes phase. Upon storing heat in the storage material, the material begins to melt when the phase change temperature is reached. The temperature then stays constant until the melting process is finished. The heat stored during the phase change process of the material is called latent heat.

Ideally, automotive engine cooling is undesirable from the thermodynamic point of view. If the heat transfer rates from the gas to metal could be reduced, then more power could be produced at a particular fuel flow rate, i.e. the thermal efficiency of the engine would increase. Also the heat removed out via radiator could be reduced and hence smaller radiator size. That is why powertrain thermal management is extremely necessary for good engine reliability and durability with a compromise of the thermal efficiency.

One of the most technically and commercially available options for this is the use of latent heat thermal energy storage system. Despite the fact that there are numerous works and reviews covering this topic, the author hopes to draw attention to some aspects of the choice of material and mathematical model for such systems.

Keywords: phase-change materials, latent heat, energy storage systems, thermal conductivity, thermo-physical properties, kinetic properties.

Introduction

Phase-change materials (PCM) are latent heat storage materials. When the source temperature increases, the chemical bonds in the PCM break up as the material transitions from solid to liquid (as is the case with solid-liquid PCMs, which are particularly relevant to the author's thesis.). The phase change is a heat-seeking (endothermic) process and therefore, the PCM absorbs heat. As heat is stored in the storage material, it melts at the phase change temperature, and until the melting process is complete, the temperature remains constant. Latent heat is the heat that remains after the material undergoes phase change (melting process) [1].

Changing the internal energy of a material can result in the storage of thermal energy, such as sensible heat, latent heat, and thermo-chemical heat, or a combination of them.

In sensible heat storage (SHS), raising the temperature of a solid or liquid is how thermal energy can be stored. During the process of charging and discharging, SHS systems make use of the material's heat capacity and temperature change. The heat stored is determined by the medium's specific heat, temperature changes, and storage material.

Latent heat storage (LHS) involves heat absorption or release when a storage material changes from solid to liquid, liquid to gas, or vice-versa. Latent heat thermal energy storage is a particularly attractive technique for thermal heat storage due to its ability to provide high energy storage density and its ability to store heat at constant temperature corresponding to the phase transition temperature of the PCM.

On the other hand, automotive ICEs are arguably the most widely used power generators. The efficiency of these systems is unimpressive, using only one-third of the input energy for propulsion. The coolant and exhaust streams both release energy into the environment in similar amounts [2]. Waste heat recovery from automotive systems is essential because there is no alternative to these ubiquitous individual power generation systems.

The use of thermal energy storage is advantageous in recovering heat from a waste stream that can be stored as latent heat in thermal energy storages (LHTS). Phase change materials are used as storage media in LHTS units, resulting in much higher energy storage capacities. Latent energy storage is facilitated by a phase change process that has an approximative isothermal behavior. The commercial usage of LHTS is still limited to sensible heat storages due to low charging and discharging heat rates, and poor thermal conductivity of the phase change material, resulting in start-up times that are impractical. Also, during phase transition, the solid-liquid interface moves away from the convective heat transfer surface, leading to an increase in thermal resistance through the solidified/melted layer.

The choice of a suitable material for the development of a LHTS-based device that facilitates starting a car engine in cold conditions, as well as the selection of an optimal mathematical calculation model, form the subject of this scientific article.

Materials and methods

When a PCM absorbs heat, it undergoes sensible heat storage until it reaches its fusion temperature, and any additional heat it absorbs is converted to latent heat for phase change.

One of the major criteria in the design of heat recovery system is the proper selection of material with optimum conditions. The extraction of heat and its storage could be achieved either by embedding the heat exchanger coil surface inside the storage tank where the storage material is present and allowed to pass through the warm water through the heat exchanger coil or providing a separate heat exchanger through which heat transferring fluid is circulated to extract heat [3].

The first step should be the selection of the PCM based on the desired melting temperature. Melting temperatures between 15 °C and 90 °C can be applied for heat leveling applications. Secondly, the selected PCM needs to present desirable thermo-physical, chemical and kinetic properties [4]. The PCM should demonstrate the congruent melting for a constant storage capacity of the material with each solidifying/liquefying

cycle as well as the high latent heat of fusion per unit volume in order to limit the required volume of the container to store the given amount of energy, while not failing to provide significant heat storage. Desired kinetic properties include high nucleating rate and high rate of crystal growth thus avoiding supercoolant of the liquid phase. The material as a chemical substance should perform reversible solidifying/liquefying cycles, do not degrade after a large number of aforementioned transformations and do not corrode the construction material either of its own container or the vehicle.

To make a meanwhile conclusion, one can say that while selecting a suitable PCM, the criteria should go as following: high latent heat of phase change, appropriate of the working temperature range, high thermal conductivity at solid state, high specific heat capacity at liquid state, good chemical stability and low vapor pressure at working temperature ranges, high density, inflammability, little volume variation during solidification, minimum thermal storing losses, environment friendly and reasonable price [5].

Results and discussions

For the low-temperature range the following PCMs are the most useful (names in brackets are given according to IUPAC nomenclature, and not trade and other commercial names): $\text{Na}_2\text{CO}_3 \cdot 12\text{H}_2\text{O}$ (sodium carbonate dodecahydrate), NaCH_3 (sodium monomethyl), $\text{CaO} \cdot 3\text{H}_2\text{O}$ (calcium oxide trihydrate), $\text{NaOH} \cdot \text{H}_2\text{O}$ (sodium hydroxide hydrate), $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ (barium hydroxide octahydrate), $\text{LiNO}_3 \cdot 3\text{H}_2\text{O}$ (lithium nitrate trihydrate) [5, 6, 7].

Thermal energy stored by thermal energy storage device can also be increased with using different PCM's having high heat of fusion. For heavy duty engine, thermal energy can be increased with increasing dimensions of thermal energy storage device [8].

Thermal energy storages using PCMs with the low thermal conductivity necessitate careful design to ensure complete melting within a desired time by choosing suitable physical geometry and dimensions. The first prototype can be developed once the most suitable PCM and proper heat exchanger are identified with potential enhancement techniques, and following stage is to numerically analyze and evaluate the prototype. The mathematical methodology should be the first step to present the melting and solidification behavior of PCM in theory.

The storage capacity of the thermal energy storage device depends on both sensible heat storage and latent heat storage. In the sensible heat storage, the energy is stored as the temperature of the storage material increases while the energy stored when a substance changes from one phase to another in the latent heat storage. The total amount of energy (Q_{stored}) stored by the storage material can be calculated by following equation:

$$Q_{\text{stored}} = m \left[\int_{T_i}^{T_l} c_{ps}(T) dT + L + \int_{T_l}^{T_f} c_{pl}(T) dT \right] \quad (1)$$

where m is the mass of material, kg;
 c_{ps} is the specific heat of material in solid phase, J/(kg·K);
 c_{pl} is the specific heat of material in liquid phase, J/(kg·K);
 L is the latent heat of solid–liquid phase change, J;
 T_i is the initial temperature of solid state, K;
 T_l is the temperature of solid–liquid phase change, K;
 T_f is the final temperature of liquid state, K.

The essential feature of the enthalpy technique [9] for convection/diffusion phase change is the latent-heat source term treatment, in the energy equation. In a system which is undergoing a change of phase under heat transfer the total enthalpy, H , may be expressed as

$$H=h+\Delta H, \tag{2}$$

where h is the sensible enthalpy, J;
 ΔH is the latent heat, J.

Latent heat storage (LHS) is based on the heat absorption or release when a storage material undergoes a phase change from solid to liquid or liquid to gas or vice-versa. The storage capacity of the LHS system with a PCM medium is given by

$$Q = ma_m\Delta h_m + \int_i^m mC_p dT + \int_m^f mC_p dt = m[a_m\Delta h_m + C_{sp}(T_m - T_i) + C_{lp}(T_f - T_m)], \tag{3}$$

where m is the mass of heat storage medium, kg;
 a_m is the fraction melted;
 Δh_m is the heat of fusion, kJ/kg;
 C_p is the specific heat, kJ/kg·K;
 C_{sp} is the average specific heat between T_i and T_m , kJ/kg·K;
 T_m is the melting temperature, K;
 T_i is the initial temperature, K;
 C_{lp} is the average specific heat between T_m and T_f , kJ/kg·K;
 T_f is the final temperature, K.

However, only a portion of stored thermal energy is available as useful heating. The rest of the energy is dissipated through the thermal losses. The useful heat (Q_{useful}) which is necessary for the heating of the engine over a temperature ΔT is determined as

$$Q_{\text{useful}} = \sum_i c_i m_i \Delta T, \tag{4}$$

where c_i is the specific heat of the engine components, J/(kg·K);
 m_i is the mass of the engine components, kg [6].

Pure substances have a single temperature of solidification, In the opposite situation, solidification occurs at different temperatures, leading to a two-phase zone (a «mushy region») [10] between the solid and liquid zones. In this latter case, it is appropriate to consider the energy equation in terms of enthalpy for the advective movements (it should be noted that although in fluid mechanics the term convection is often used as a synonym instead of the term «advection», many authors and engineers try to use the word «convection» to describe transport through molecular and eddy diffusion, while «advection» denotes the overall flow of fluid [in a pipe or channel]).

The solution of this equation problem requires knowledge of the enthalpy–temperature functional dependency. Similarly, it is necessary to know the function relating the thermal conductivity and the temperature.

The main advantages of this method are that the equation is directly applicable to the three phases, the temperature is determined at each point and the value of the thermo-physical properties can be evaluated, and finally, according to the temperature field, it is possible to ascertain the position of the two boundaries if so desired, although as indicated above this is not necessary.

Conclusions

Latent heat storage system is a good device, which offers the following benefits:

- higher heat capacity;
- isothermal charging and discharging;
- variation in the surface heat transfer rate due to poor thermal conductivity of phase change material is minimized;
- compact size;
- economical operation.

If all the conditions for a competent and rational choice of material for the latent heat accumulation system are met, mathematical calculations show the following:

1. Regardless of load conditions, the effectiveness of these systems reaches its peak at the end of the charging process.
2. The system is capable of recovering nearly fifteen hundredths of total heat that would otherwise be wasted in the atmosphere.
3. By lowering the temperature of the heat transfer fluid below 90 °C, heat can be extracted more efficiently.
4. Heat is transferred in the axial direction of the storage tank by conduction due to the presence of the container and the high conductivity storage wall, thus, no stratification and a temperature that is almost uniform throughout the tank are observed.

Both the charging rate and charging efficiency are very high at higher load and they decrease with respect to load, as seen on Fig. 1. In order to recover the maximum amount of heat, a cascaded latent heat storage system with multiple PCM is suggested and this concept is presently under investigation.

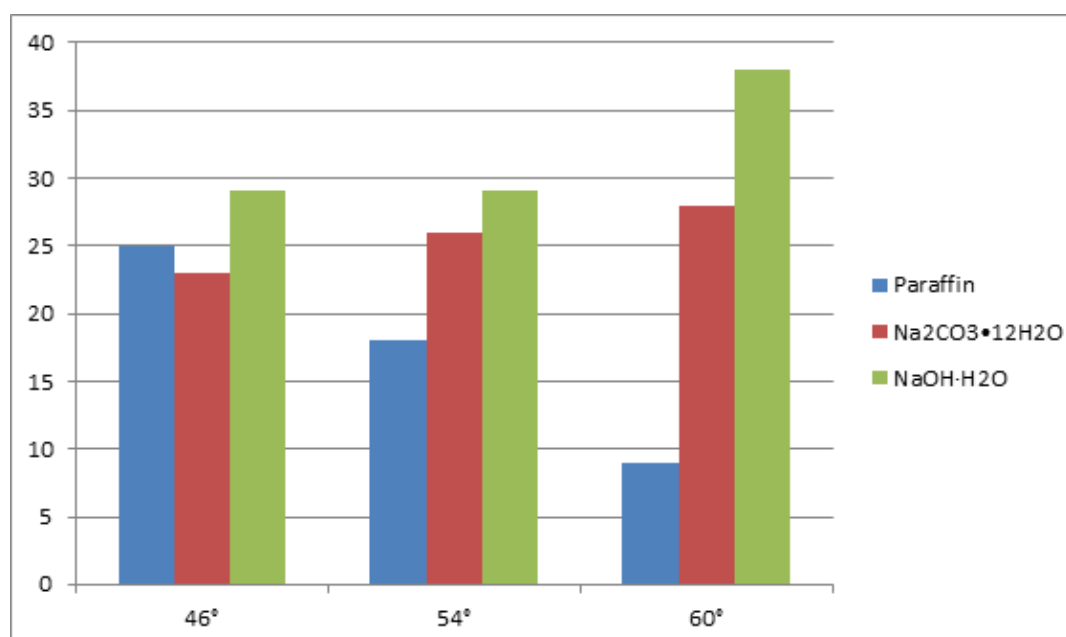


Figure 1 – Phase change enthalpy (in $\text{kJ} \cdot \text{kg}^{-1} \cdot ^\circ\text{C}^{-1}$) for different phase change materials.

At higher load, both the charging rate and charging efficiency are very high, but they decrease depending on the load. To maximize heat recovery, a latent heat storage system with multiple PCM can be suggested, and this concept is of a significant interest to explore further.

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Accepted for publication 07.12.23

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Басып шығаруға 07.12.23 қабылданды.

АВТОКӨЛІКТІҢ ЖАСЫРЫН ЖЫЛУ САҚТАУ ЖҮЙЕСІ ҮШІН ФАЗАЛЫҚ ӨЗГЕРТУ МАТЕРИАЛЫ ЖӘНЕ МАТЕМАТИКАЛЫҚ МОДЕЛІН ТАҢДАУ

Фазалық ауыспалы материалдар жасырын жылу сақтайтын материалдар болып табылады. Көздің температурасы көтерілген сайын, материал фазасы өзгерген кезде фазалық ауыспалы материалдар ішіндегі химиялық байланыстар үзіледі. Материалына жылулы жеткізу сақтай отырып, фазаның өзгеруі температурасына жеткенде материал ери бастайды. Содан кейін температура балқыту процесі аяқталғанша тұрақты болып қалады. Материалдың фазалық өзгеру процесінде жинақталған жылу жасырын жылу деп аталады.

Ең дұрысы, автокөлік моторын салқындату термодинамикалық тұрғыдан қажет емес. Егер газдан металға жылу беру жылдамдығын төмендетуге болатын болса, онда белгілі бір отын ағыны жылдамдығында көбірек қуат өндіруге болады, яғни қозғалтқыштың жылу тиімділігі артады. Сондай-ақ радиатор арқылы шығарылатын жылуды азайтуға, демек, радиатордың өлшемін азайтуға болады. Сондықтан қозғалтқыштың жақсы сенімділігі мен жылу тиімділігін төмендететін ұзақ мерзімділігі үшін қуат блогының жылуын басқару өте қажет.

Бұл үшін техникалық және коммерциялық қол жетімді нұсқалардың бірі жасырын жылу жылу энергиясын сақтау жүйесін пайдалану болып табылады. Осы тақырыпты қамтитын көптеген жұмыстар мен шолулар бар екеніне

қарамастан, автор мұндай жүйелер үшін материалды және математикалық модельді таңдаудың кейбір аспектілеріне назар аударуға үміттенеді.

Кілтті сөздер: фазалық ауыспалы материалдар, жасырын жылу, энергия сақтау жүйелері, жылу өткізгіштік, термофизикалық қасиеттер, кинетикалық қасиеттер.

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Принято к изданию 07.12.23.

ВЫБОР ПОДХОДЯЩЕГО МАТЕРИАЛА С ФАЗОВЫМ ПЕРЕХОДОМ И МАТЕМАТИЧЕСКОЙ МОДЕЛИ ДЛЯ АВТОМОБИЛЬНОЙ СИСТЕМЫ АККУМУЛИРОВАНИЯ ЛАТЕНТНОЙ ТЕПЛОТЫ

Материалы с фазовым переходом (МФП) аккумулируют скрытую теплоту. По мере повышения температуры источника тепла химические связи внутри МФП разрушаются, поскольку имеет место фазовый переход. При сохранении теплоподвода материал начинает плавиться по достижению температуры фазового перехода. Затем температура остается постоянной до тех пор, пока процесс плавления не завершится. Тепло, запасаемое в процессе фазового перехода материала, называется скрытой теплотой.

В идеале охлаждение автомобильного двигателя нежелательно с термодинамической точки зрения. Если бы можно было снизить скорость теплопередачи от топливных паров к металлу, то при определенном расходе топлива тепловой КПД двигателя увеличился бы. Однако можно уменьшить тепло, отводимое через радиатор, и, следовательно, уменьшить размер радиатора. Поэтому управление температурным режимом силовой установки крайне необходимо для обеспечения надёжности и долговечности двигателя.

Один из наиболее доступных технически и коммерчески вариантов решения данной проблемы — это применение систем аккумулирования латентной теплоты. Несмотря на то, что существуют многочисленные работы и обзоры, затрагивающие эту тематику, автор надеется обратить внимание на некоторые аспекты выбора материала и расчётной математической модели для таких систем.

Ключевые слова: материалы с фазовым переходом, скрытая теплота, системы накопления энергии, теплопроводность, теплофизические свойства, кинетические свойства.

Теруге 08.12.23 ж. жіберілді. Басуға 29.12.23 ж. қол қойылды.

Электрондық баспа

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