Compact latent heat storage decarbonisation potential for domestic hot water and space heating applications in the UK

Jose Pereira da Cunha⁎, Philip Eames

Loughborough University, Wolfson School of Mechanical, Electrical and Manufacturing Engineering, Loughborough, Leicestershire LE 11 3TU, United Kingdom

HIGHLIGHTS

• PCM store with air source heat pump comparison to gas boiler for DHW and SH.
• Both systems integrated into semi-detached dwelling in typical UK midlands climate.
• PCM store system reduced yearly CO2 emissions by 56% and consumed 76% less energy.
• PCM store system LCOE was 117.84£/MWh, compared to 69.66£/MWh for the gas boiler.

ARTICLE INFO

Keywords:
Phase change materials
Latent heat thermal storage
Domestic hot water
Domestic space heating
Air source heat pumps, finite volume enthalpy models

ABSTRACT

A performance comparison is presented for a domestic space and hot water heating system with a conventional gas boiler and an air source heat pump (ASHP) with latent heat storage, both with solar thermal collectors for a typical UK climate, to demonstrate the potential of phase change material based energy storage in active heating applications. The latent heat thermal storage system consisted of 10 modules with RT54HC comprising a total storage capacity of 14.75 kWh that provided 53% extra thermal storage capacity over the temperature range of 40–65 °C compared to a water only store. The simulations predicted a potential yearly CO2 reduction of 56%, and a yearly energy reduction of 76% when operating the heat pumps using the economy 10 electricity tariff i.e. a low tariff between 00.00 and 05.00 and 13.00–16.00 with current grid emission values compared to the conventional gas boiler system; successfully offsetting the electrical load to meet the required heat demand. Due to the high capital costs of the heat pump system with latent heat storage, its levelized cost of energy was 117.84£/MWh, compared to 69.66£/MWh for the gas boiler, on a 20-year life cycle.

1. Introduction

Approximately 18% of the UK’s final energy consumption in 2016 was used for domestic water heating, mainly through the use of natural gas boilers [1], totalling 26773 mtoe. In order to decarbonize the sector, the use of renewable heat sources such as solar thermal could be implemented, backed up by either heat pumps or gas boilers. Heat pump operation should, where possible, be restricted to off peak times to prevent an increase in the peak electrical grid demand [2].

Fig. 1 presents the UK national grid emissions on each season of 2016 [3]. The CO2 emissions associated with each generation profile were calculated based on the emission coefficients obtained by Hawkes [4].

To effectively decarbonize this sector, heat pump CO2 emissions should be less than the currently used conventional gas burning domestic heating systems (around 204 g CO2/kWhth [4,5]), and operated during off peak electrical load times to minimise both carbon intensity and peak electrical load. This can be achieved if heat pumps are operated using either economy 10 or economy 7 electricity tariffs [5], with hot water buffer tanks used to store heat, offsetting the electrical load while meeting the heat demand required.

The higher CO2 grid emissions during the winter months are mainly due to the higher consumption of coal and natural gas, consequence of a larger electrical demand by the UK grid. It can be seen in Fig. 1 that the lowest CO2 daily emission period is from 23.00 to 05.00 and a depression in the marginal emissions curve occurs from 12.00 to 16.00 in all seasons.

Hot water tanks have nearly constant heat capacity over the working temperature range of 40–65 °C [6], typical temperature band for domestic hot water and space heating, hence requiring a considerable volume to buffer some of that daily heat demand.
2. PCM screening and characterization

Phase change materials (PCMs) with a phase transition temperature between 50 and 60 °C can effectively be used to increase thermal storage capacity in that narrow temperature range, hence reducing the required storage volume achievable with hot water buffer tanks. Commercial organic PCMs melting in this temperature range are Paraffin waxes (RT52, RT54HC [7]) and fatty acids, such as the eutectic mixture of stearic and palmitic acids (36/64%wt) studied by Baran and Sari [8]. Salt hydrates are other candidate PCMs, however their high subcooling were prepared experimentally and their specific heat capacities and using the resolution of the slower ramp rate

The parafln wax RT54HC, the eutectic mixture of stearic acid-palmitic acid [8] (36/64%wt) and the eutectic mixture of magnesium nitrate hexahydrate and magnesium chloride hexahydrate (41/59%wt) were prepared experimentally and their specific heat capacity determined using differential scanning calorimetry (DSC). Table 1 presents the thermophysical properties of the 3 PCMs characterized. It can be seen that the salt hydrate eutectic mixture is nearly 3 times more energy dense than the same volume of water, within the 40–65 °C temperature range.

The heat capacity thermograms presented in Fig. 2 were determined experimentally using the TA instruments Discovery differential scanning calorimeter [16] at 2 different temperature ramp rates, 1 and 10 °C/min [17], using the faster ramp rate as reference for the solid and liquid heat capacities and using the resolution of the slower ramp rate for the thermogram.

3. Developed numerical model

A 2D finite volume model was developed to simulate a compact latent heat energy storage system, similar to the tubular array studied by Nakaso et al. [18] in Matlab. The numerical model assumed isotropic heat propagation within the PCM, having temperature-dependent thermal conductivity and volumetric heat capacity [J/m3 K] with no volume changes occurring during phase change.

The compact tube-in-tube simulated a long copper string inserted into a rectangular PCM slab, as illustrated in Fig. 3A. In order to meet the required storage capacity, the model added numerous strings in parallel connected through a larger diameter copper manifold pipe, distributing the water flow evenly throughout the multiple strings, seen schematically in Fig. 3B. The model employed backward spatial discretization for the water flow, and unidirectional radial and axial heat propagation among the copper tube and PCM, as it is presented schematically in Fig. 3C and D.

The container’s heat loss to ambient was accounted to the last PCM node outer surface, determined using the insulation properties specified in the container (insulation thickness, type and ambient temperature) and divided by the number of axial nodes and strings. The simulated charge and discharge of the container represented a fluid flowing in the inner tube, exchanging heat by convection with the tube inner surface.

The Heat Transfer Fluid (HTF) Reynolds number was calculated using Eq. (1), for pipe flow. For laminar flows, the average Nusselt Number was obtained considering a constant wall temperature, according to the correlation from [19], expressed in Eq. (4). For fully turbulent flows, with a Reynolds number above 10,000, Nusselt numbers were obtained with the correlation put forward by Gnielinski [19], expressed in Eq. (5). For transitional flows, a linear interpolation (Eq. (3)) between the laminar and turbulent regimes was adopted, Eq. (2).

The developed numerical model calculated new mass and transport matrices at each time step to enable the transient accounting for changes in the PCM’s heat capacity (phase change) and thermal conductivity.

Some of water’s thermophysical properties (namely viscosity and the Prandtl number) were also temperature dependent, due to the
changes in the convective heat transfer coefficient. The spatial discretization, seen in Fig. 3C and D, employed 9 radial nodes and 40 axial nodes giving a modelled cylinder height to thickness ratio between 125 and 170.

Eq. (6) presents the three sets of equations used to compute the solution during each time step ([Γ'] the transport matrix, [C] the mass matrix, \( f_t \) is a variable ranging from 0 to 1 that can be used to tune the algorithm from an explicit to an implicit approach), all models were solved implicitly. The term \( \{F_{out}\} \) accounts for the inlet mass flow.

\[
\begin{align*}
\{I_2\} &= f_t \cdot \{I_1\} + [C] \\
\{m_t\} &= (1-f_t) \cdot \{I_1\} \times [T_{old}] + [C] \times [T_{old}] + \{F_{in}\} \\
\{T_{new}\} &= \{I_2\}^{-1} \times \{m_t\}
\end{align*}
\]  

(6)

3.1. Model verification

A compact latent heat storage module was developed in situ to investigate the thermal performance of PCMs in a rectangular slab. The rectangular slab was made from 3 mm aluminium sheet bolted to four 1.5″ aluminium profiles. A ½″ copper pipe string was inserted within the slab to exchange heat between the water flow and the PCM. The copper string comprised 39 U-bends soldered to 511 mm tube sections. Copper metal fins were soldered to the tube outer surface to improve heat transfer among the PCM. A simplified view of the rig is displayed in Fig. 4A.

The rectangular storage contained 18.3L of RT44HC [7], able to store 1.39kWh when heated/cycled from 20 to 70 °C. The storage general dimensions and main characteristics are presented in Table 2. Water is used as the heat transfer fluid, while the PCM (RT44HC [7]) occupies the spaces around the pipe within the rectangular tank. The PCM slab is inserted within a 12 mm thick MDF enclosure (thermal conductivity 0.151 W/m K) with 20 mm air gaps between the container sides, as seen in Fig. 4B. Using 5 copper fins spaced 32 mm and soldered transversally to the copper pipe increased the total heat transfer area within the PCM by 52%.

A Huber Unistat tango was used to indirectly exchange heat with the water rig, using a programmable proportional-integral-derivative (PID) controller to maintain the set point temperature constant during charging and discharging the store. Thermocouples are fixed at the HTF inlet and outlet of the thermal store. The PCM temperature is monitored using thermocouples positioned at the 2 locations presented in Fig. 4A, and the flow rate is monitored by a turbine flow meter from Icenta, its signal converted to current and read in a compact DAQ card from

| PCM | \( \Delta T \) °C | \( \text{H}_{\text{stored}} \) kWh/m³ | \( \text{H}/\text{H}_{\text{LCO}} \) kWh/kWh | \( \lambda \) mW/m K | Price £/kWh |
|-----|-----------------|-----------------|-----------------|-----------------|-----------------|
| 41%MgCl₂·(H₂O)₆ + 59%Mg(NO₃)₂·(H₂O)₆ (SH-SH) | 40-65 | 78 | 2.72 | 600 | 606 | 1.19 [9,10] |
| 36%stearic acid + 64%palmitic acid (SA-SPA) [8] | 61 | 2.11 | 288 | 168 | 5.72 [11,12] |
| RT 54HC [7] | 52 | 1.80 | 215 [13] | 165 [14] | 7.63 [15] |

Table 1

Properties of PCMs selected for potential use in space heating applications.

Fig. 2. Heat capacity thermograms for the three selected PCMs determined experimentally at a ramp rate of 1 °C/min.
The experiment is carried out in two modes: charging and discharging. For the charging mode, the initial state of the PCM is solid at room temperature of 20.3 °C. The HTF is heated in the shell and tubes heat exchanger and pumped through the copper pipe. The charging is completed when all the PCM in the tank has melted fully and its temperature has stabilized around 70 °C, with temperature readings taken every minute. For the discharging mode, the HTF temperature is dropped to 20 °C and temperature readings continue until the PCM temperature has stabilized around 20 °C. Fig. 5 presents the comparison between experimental results and modelled numerical results obtained for the temperature profiles. The thermal store had fully melted at 180 min, as can be seen in Fig. 5.

Fig. 6 presents the comparison between the experimental results and modelled simulation results obtained for the heat rate profiles. The PCM’s conductivity increase has negligible effect in the water flow inlet/outlet temperature difference, mainly because the driving buoyancy force is nearly suppressed, with both predictions following the experimental results accordingly.

3.2. System design and integration

Following the parametric analysis, the latent heat store was integrated into a simulation of a domestic heating system, illustrated schematically in Fig. 7. An air source heat pump was used as the heat source, working during off peak hours based on economy 10 electricity.
The latent heat system was sized to meet the highest heat demand for a semi-detached dwelling over a period of 8 h during the predicted simulation for winter conditions, with paraaffin wax RT54HC [7]. The reason for using paraaffin wax as the PCM was due to the developed numerical model being verified for a similar wax. The building fabric thermal performance was considered improved by insulation retrofit compared to a conventional 1930 semi-detached dwelling. The reason for selecting this type of dwelling is due to its importance, since it represented a quarter of the British housing stock in 2015, around 6 million dwellings, based on the English housing survey report made by the Department for Communities and Local Government [22].

The 80L hot water tank would be charged in off peak hours with the circulating pump P1 (20 L/min maximum). If the solar thermal collector temperature was 1 °C above the hot water tank, the solar circulator pump P3 (2 L/min per collector) would directly charge the hot water tank, as presented in Fig. 7. The reason for using a small hot water tank would be to compensate the temperature drop of the latent heat store in periods of high heat demand consequence of having a low water volume within the latent heat store.

The household space heat distribution system would be met by circulating pump P2 (12 L/min) transferring heat directly from the hot water tank to the household, shown schematically in Fig. 7. When indoor temperature dropped 0.5 °C below the set point, P2 would be activated until it achieved an indoor temperature 0.5 °C above the set point. Whenever a hot water appliance was activated, valve V1 would open and thermostatic valve Vt would regulate the hot water flow coming from the hot water tank to maintain a constant 38 °C temperature output.

**Table 2**

| Store dimensions, heat transfer fluid and storage material properties for the experimental work performed. |
|---|---|---|
| PCM slab width [mm] | 600 | Volume [L] | 21.3 |
| PCM slab length [mm] | 950 | PCM volume [L] | 19.0 |
| PCM slab thickness [mm] | 37 | Number of fins | 18 |
| Coil length [m] | 12.14 | PCM fraction [%] | 88.9 |
| Tube OD (ID) [mm] | 15.86 (12.45) | Specific HT area [m²/m³ PCM] | 48.23 |
| HTF (average values): | | | |
| Flow rate [g/s] | 148.10 | Hₜ (37–46 °C) [KWh/m²] | 49.57 |
| Re | 24 603 | Cₚ (20–37 °C) [MJ/m² K] | 1688.4 + 1.6211 * T |
| Pr | 4.28 | Cₚ (46–70 °C) [MJ/m² K] | 1323.5 + 9.7665 * T |
| Nu | 153 | λₜ (20–37 °C) [W/m K] | 0.450 – 0.00096 * T |
| (hcv) [W/m² K] | 72.49 | λₜ (46–70 °C) [W/m K] | 0.188 – 0.00036 * T |

**Fig. 4.** Experimental rig used with RT44HC [7] and simplified view of the thermocouples and flow meter distribution.
The convective heat transfer coefficient of the heat emitters (Eq. (11)) was determined during each time step by calculating the Rayleigh number (Eq. (9)) and Nusselt coefficient for a vertical surface (Eq. (10)) using the instantaneous emitter-ambient temperature difference, and considering a typical emitter height of 600 mm [6]. The radiative heat transfer coefficient, assuming the heat emitter area much smaller than the household's walls and a surface emissivity of 0.95, can be calculated according to Eq. (12) using also the instantaneous emitter-ambient temperature, from [19]. The emitter global heat transfer coefficient, seen in Fig. 8D and E, would be the sum of the two coefficients, seen in Eq. (13). The convective heat transfer coefficient is multiplied by 2 since convection occurs on the 2 sides of the heat emitter.

\[
Ra(t) = \frac{g \times \rho \times h^4 \times (\frac{T_{amb}(t) - T_{emitter}(t)}{\overline{T}_{emitter}})}{\xi^2} \times \rho_0
\]

(9)

\[
Nu_{air} = \left\{ 0.825 + 0.387 \left( Ra \left[ 1 + \left( \frac{0.492}{Fr} \right)^{0.5} \right] \right)^{0.5} \right\}^{0.2}
\]

(10)

\[
h_{conv} = \frac{Nu \times \lambda_{air}}{L_{emitter}}
\]

(11)

\[
h_{rad} = \varepsilon_{emitter}(T_{amb}^4 + T_{emitter}^2)(T_{amb} + T_{emitter})
\]

(12)

\[
U_{A_{emitter}} = A_{emitter}(2 \times h_{conv} + h_{rad})
\]

(13)

The designed latent heat storage module developed was able to store 255L of PCM material with 10 strings connected in parallel. Using off-the-shelf copper pipe accessories, each string had a 11.56 m ½" nominal size copper tube string, with 37 U-bends, as presented in Fig. 9A. All 10 strings would then be connected to a larger copper manifold, ensuring an even flow distribution, as seen in Fig. 9B.

With the RTS4HC [7] (properties summarized in Table 1), occupying around 67% of the total storage system volume, its total thermal energy storage capacity increased by 53% compared to the same store volume using only water, between 40 and 65 °C, due to the latent heat capacity of the PCM between 52 and 56 °C, as shown in Fig. 2. Table 4 presents the geometrical properties of the modelled latent heat storage. Using 18 fins per string increased the specific heat transfer area by 387%.

Having 10 strings within the store allowed the heat transfer fluid flow to be divided by the same factor in the ¾" manifold pipe, as it can be seen in Fig. 9B. That would result in reducing the Reynolds number when charging from the heat pump from 30,000 (fully turbulent) to 5800 (turbulent), reducing subsequently pipe head losses from 54 kPa to 63 Pa.

4. Results

Fig. 10 presents the predictions of heat supplied for the dwelling in a winter and summer day, using McKenna’s high-resolution stochastic model [21].

In these simulations, there is a significant variance in the dwellings indoor temperatures around the set point temperatures, consequence of having wider boiler set point temperatures (varying from 15.1 to 24.4 °C for the winter climate predictions). During spring, summer and autumn months, the solar thermal collector temperature went above 100 °C due to having the DWH tank cut off temperature at 70 °C and insufficient thermal capacity to store available daily solar energy below 70 °C, leading to a significant loss of solar thermal energy.

The predicted temperatures and heat supply rates from simulations using the developed model are presented in Fig. 11.

This model predicts more rapid indoor temperature variations mainly resulting due to the narrow temperature control band (± 0.5 °C), which leads to more variations in the heat emitter temperatures.
It can be seen that the heat pump operates mainly during the winter months due to low solar radiation, being the required thermal energy provided almost entirely by the solar thermal collectors in the remaining months, due to the system’s higher thermal storage capacity. The big temperature variations in the latent heat store mainly in the cold end side is consequence of its low water volume within the store (only 16 L) dropping steeply whenever a cold temperature inlet is presented either by the heat emitters of the grid water. It can also be seen the PCM effect on the store’s cold temperature rising steadily and converging near the PCM’s melting point of 54 °C when there’s no hot water consumption of no circulation through the heat emitters. Considerable thermal stratification was successfully achieved mainly due to the solar thermal input, proving to be beneficial when comparing with the conventional system from Mckenna’s model [21].

The winter climate predictions demonstrated that the higher thermal capacity around 54 °C of the PCM allowed the latent heat store
system modelled by Mckenna.\footnote{For interpretation of color in Fig. 12, the reader is referred to the web version of this article.}

Energy consumption was 79% less than the conventional gas boiler\cite{23}. The seasonal CO2 emissions were calculated in the conventional system by multiplying the energy used in the gas boiler each day with the associated emissions of natural gas from \cite{4}, divided by the boiler efficiency (estimated to be 85%\cite{24}).

The seasonal CO2 emissions were calculated in the conventional system by multiplying the energy used in the gas boiler each day with the associated emissions of natural gas from \cite{4}, divided by the corresponding grid emission values\cite{1,4} for the heat pump systems with stores was 62% less. The obtained values could have been more promising using the salt hydrate eutectic mixture; however, corrosion and material segregation issues might limit the storage cycle reversibility\cite{25}.

4.1. Economical comparison of all modelled systems

In order to estimate a simple payback period for a 20 year life span, a market assessment was made to all the required components to install the proposed systems. In terms of heat source, Table 5 presents the capital difference cost of installing an air-source heat pump unit with solar thermal collectors to the conventional gas boiler unit. Based on the studies performed by Kelly et al.\cite{26}, installation costs were considered 5% of the initial capital expense (CAPEX) and operation and maintenance 1% of the initial CAPEX.

Table 5 also presents a general comparison for storage costs. For the hot water tank pricing, prices were retrieved from Mibec thermal solutions\cite{33}, and a linear interpolation defined the value for the specific volume in question. The compact latent heat storage presents a higher CAPEX, mainly due to requiring a considerable amount of copper tubing and solder fittings.

Table 6 presents the levelized cost of energy (LCOE) for each solution according to dwelling size. Eq. (14) presents the procedure used to determine, for a lifetime of 20 years\cite{35} and an interest rate of 3.5%, the LCOE for each system (assuming a “zero-risk” investment), based on Smallbone et al.\cite{35}. Gas and electricity (economy 10\cite{5}) prices were retrieved from SSE\cite{36}. Ecology 10 electricity tariff considered was 8.46p/kWh and gas tariff was 3.72p/kWh, both with a daily standing charge of 14.8 pence.

\[
LCOE = \frac{\text{CAPEX} \times \left(1 + \frac{r}{(1+r)^n}\right) + \text{OPEX} + Q_{\text{usable}} \times F_{\text{tariff}}}{\text{Heat production} \times n} \times 1000 \left[ \frac{\text{£}}{\text{MWh}} \right]
\] (14)

It can be seen that the LCOE for all storage systems reduces with increasing storage capacity; packed beds offer the lowest among the 3 storage solutions studied. Although the buffer tank presents the lowest CAPEX among the storage solutions studied, its LCOE is still higher than the other two storage solutions due to its lower energy savings. Gas boilers at current gas prices are still the most economical option, however they match the LCOE of packed bed if a carbon tax of 8.85£/ton is added to its fuel price, value still below the estimated by Brink et al.\cite{37} of around 17£/ton for 2016.

Assuming the 11.54£/tonCO2 applied to current natural gas boilers,
value still below the assumed 17£/ton by the UK government [38], the payback was calculated for the replacement of current natural gas heating system using Eq. (15). To obtain a payback period of 8 years, the heat pump system would require a CAPEX reduction of 52%.

\[
\text{CAPEX} \times r \left( \frac{1}{1 + r} \right)^{\text{payback}} = \frac{\text{Savings}_{\text{year}} \times \text{OPEX}}{\text{CAPEX} \times r \left( \frac{1}{1 + r} \right)^{\text{payback}}} - Q_{\text{use}} \times E_{\text{eff}}
\]

(15)

5. Conclusions

Thermal stores including phase change materials have the potential to store larger amounts of thermal energy within a smaller temperature range compared to stores just using water. Due to the low thermal conductivity of many PCMs, poor rates of thermal diffusion within the PCM can reduce significantly the nominal storage system charge and discharge heat transfer rates.

Modifying the store geometry by allowing a parallel flow configuration among the latent heat storage modules reduces the flow passing through each module allowing a bigger thermal stratification.

The numerical model developed to evaluate the replacement of conventional gas fired boilers with heat pumps coupled with a PCM thermal store to offset heat pump operation from peak electrical demand periods in a semi-detached dwelling, predicted that yearly CO2 emissions could be reduced by an average of 58% using current grid emission values. Accounting that these type of dwelling represents 25% of the British housing stock, a 58% reduction emission on these dwellings would represent a yearly reduction of 8.64 million tonnes of CO2 if the system was integrated in the 6 million semi-detached dwellings in the UK, values that would increase if further efforts to decarbonize UK’s electrical grid are taken.

Economically, the integration of PCM’s into domestic hot water systems is a costly solution, using current energy prices, being the best levelized cost of energy obtained for heat pump with compact latent heat store 117.84£/MWh. A carbon tax to current natural gas consumption of 8.94£/ton CO2 is required to equal the levelized cost of energy of natural gas to the latent heat storage system, for a 20 years life cycle value still below the assumed 17£/ton CO2 by the UK government for 2016. If the initial capital expense is backed 33% by the
government, the heat pump system would payback itself in 8 years (assuming a carbon tax of 11.54 £/tonCO2 emitted for the gas boiler).

To meet the UK’s 80% carbon emissions reduction targets by 2050, the electrification of current domestic water heating systems must be made. The increased peak electrical load generated by the electrification of heat can be moderated by using enhanced buffer tanks with their thermal capacity increased by including PCMs to allow operation of heat pumps to be time shifted to periods of low grid electrical load while still meeting heat demand and comfort requirements.

Acknowledgements

The research presented in this paper is funded by the EPSRC through Grant reference EP/K011847/1, the Interdisciplinary centre for Storage, Transformation and Upgrading of Thermal Energy (i-STUTE) and a Loughborough University funded PhD studentship.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.applthermaleng.2018.01.120.

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