An Improved Model For Phase Change Material (PCM) Thermal Storage Tanks

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Abstract

This work, performed in the context of the LowUP H2020 European project, presents a modelling approach for a PCM thermal storage tank. This model will allow estimating the potential of Latent Thermal Energy Storage technologies to support efficiency improvements in novel integrated heating and cooling solutions. Here, an existing modelling approach from literature is improved focusing on the mathematical representation of the PCM and its associated non-linear behavior. Main modelling assumptions are based on an energy balance for the PCM (assuming homogeneous temperature), the by-pass factor accounting for heat transfer inefficiencies and a simple representation of the phase change process through reasoned parametrization of the h-T curve. Finally, the new proposed model is implemented into a custom TRNSYS Type and validated through satisfactory comparison between simulated and experimental values for several literature test cases.

Keywords: Thermal Energy Storage, Phase Change Materials (PCM), mathematical model, TRNSYS.

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1. Background

Phase Change Materials (PCM) for heating and cooling applications in buildings have experienced an important growth in recent years. Particularly, numerous works investigating thermal energy storage solutions for low and medium temperature applications can be found in literature (da Cunha and Eames 2016). Scientific efforts have been recently centered on development of mathematical models to be applied in simulation analyses (Verma and Singal 2008), while several studies focused on experimental research related to this kind of systems, which constitute interesting data sources for validation of mathematical models (D'Avignon and Kummert 2016, Torregosa-Jaime et al. 2013). Special attention should be paid in this sense to the modelling research conducted by Belmonte et al. (2016). They presented a simple model for Thermal Energy Storages (TES) containing PCM. It is based on the traditional bypass factor method to obtain a simple representation of generic PCM storages that can be particularly suitable for application during preliminary design stages.

The purpose of this work is to develop and present an improved model for PCM thermal storage tanks based on a modified approach of the model from Belmonte et al. (2016). The proposed model will be validated with experimental data from literature and then implemented in a TRNSYS (Klein et al. 2009) .dll file to be available for use in future extended energy analyses.

2. Modelling approach

The simplified approach from literature is based on the application of an energy balance to a PCM-based TES system with homogeneous temperature taking into account the energy transferred from/to the heat transfer fluid (HTF) and the storage heat losses. The method considers the first term in any PCM-based storage system as though a portion of the HTF ideally transfers its entire heat content to the PCM, whereas the remainder by-passes the TES system unchanged. This bypass factor stream represents the heat transfer inefficiencies between the HTF and the PCM and through the PCM itself, which will occur during a real process in a TES system. This enables simple representation of the heat transfer phenomena using only a few parameters, which is an advantage for manufacturers and designers as well as for implementing the model into simulation or energy analysis tools. Further details can be found in the original paper, and are omitted here for the sake of simplicity.

The aforementioned main concept from the original model from Belmonte et al. (2016) also constitutes the basis of the approach here proposed. However, previous results from the original model and its prediction capabilities were analysed in more depth leading to the identification of potential improvements. In particular, this work addresses the following aspect: the original approach assumed that the PCM of the storage tank melts and freezes at a

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constant temperature, which is not strictly true for most of the existing PCMs being used in building conditioning applications. This leads to most of the observed differences between simulated and experimental data for Belmonte’s work.

The new PCM storage modelling approach corrects this limitation though a more detailed representation of the PCM thermodynamic behaviour (enthalpy-temperature curve or h-T curve, see Fig.1), particularly in the phase-change temperature range.

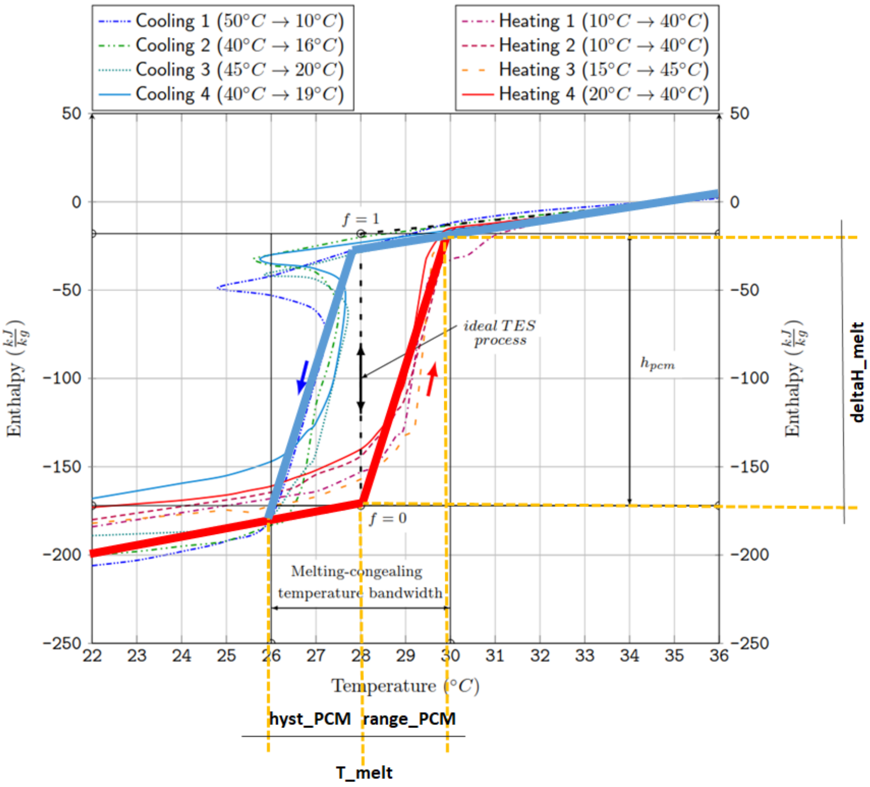

Fig.1: h-T behaviour of PCM and definition of related model parameters. Modified from Belmonte et al. (2016)

The actual behavior of PCMs often presents important deviations from the the simplified original assumption of constant melting temperature. These can be associated to the following three main different effects, which are also shown in the example h-T curves in Fig.1 representing real loading and unloading cycles of a given PCM:

- Variable temperature along the phase change process (temperature range)
- Different h-T curves (within the phase change range) for cooling and heating evolutions (i.e. hysteresis effects)
- Subcooling effects that makes the PCM requiring to achieve colder temperatures than the expected melting temperature range in order to start solidification (therefore, once the freezing process starts, the temperature increases slightly).

Depending on the level of detail applied to the modelling of the PCM thermo-physical behaviour, different approximations to represent the real h-T curve could be used. This work proposes a PCM model based on the definition of 3 parameters to specify the h-T characteristic of the material, which allows accounting for most of common h-T behaviours with reasonable accuracy:

- The melting temperature (T_melt): it is here defined as the temperature at which the PCM starts melting during a heating cycle starting from completely solid state.
- The melting range (range_PCM): it is defined as the temperature range comprised between the melting temperature and that thermal level at which all the material in solid state disappears during a heating cycle starting from completely solid state (i.e. the temperature that indicates the completeness of the solid-to-liquid transformation)
- The melting hysteresis (hyst_PCM): it is defined as the temperature difference between the two limiting states at which the material is completely in solid phase during a heating cycle (starting from completely solid material) and a cooling cycle (starting from completely liquid material). In both cases, other states obviously

correspond to completely solid material, however the referred two limiting states consider that any differential temperature increase would imply the co-existence of solid and liquid phases.

In addition, it should be noted that subcooling effects are neglected by this model. A clearer graphical definition of these parameters is also depicted in Fig.1.

Consequently, the main characteristics of the improved model are as follows:

- PCM storage volume treated as a thermal storage with homogeneous temperature.
- Improved parametrization of the enthalpy-temperature (h-T) behaviour of the Phase Change Material based on 3 parameters: melting temperature, melting range and melting hysteresis.
- Energy content of the PCM storage calculated through direct application of energy balance and according to the bypass concept to account for heat transfer inefficiencies.

The corresponding equations were programmed in MATLAB environment as a proof of concept and further implemented in a new dedicated TRNSYS Type.

Table 1 collects all the model inputs, outputs and internal variables required for the application of the proposed PCM storage model.

Table 1. Model inputs, outputs and internal parameters for the PCM storage model

Model Inputs	
T_ini_TES	Initial temperature of the PCM storage
m_s	Source massflow rate
m_l	Load massflow rate
T_si	Inlet temprature of the source flow
T_li	Inlet temperature of the load flow
T_room	Room temperature (temperature of the PCM tank surroundings)
V_PCM	Volume capacity of the PCM storage tank
A_TES	Tank surface area in contact with surroundings temperature
U_loss	Total tank heat loss coefficient
phi	Fraction of total TES volume filled with PCM
FB	Bypass factor
Model Outputs	
T_PCM	Temperature of the PCM storage
E_PCM	Energy level of the PCM storage
Q_loss	Heat transfer losses through PCM tank surface
T_so	Outlet source temperature
T_lo	Outlet load temperatue
Q_s	Heat transfer to the source flow
Q_l	Heat transfer to the load flow
f	Melted fraction of PCM (0 = completely solid; 1 = completely liquid)
Internal Parameters	
U_loss	Overall heat transfer coefficient from the PCM layer to the ambient temperature (including insulation and convective/radiant external thermal resistance)
Rho_PCM_liq	Density of the PCM liquid phase
Rho_PCM_sol	Density of the PCM solid phase
Cp_PCM_liq	Specific heat capacity of the PCM liquid phase
Cp_PCM_sol	Specific heat capacity of the PCM solid phase
deltaH_melt	Specific enthalpy
Range_PCM	Characteristic temperature range for the phase change process
Hyst_PCM	Characteristic temperature hysteresis for the phase change process

3. Results and discussion

The proposed model was validated based on 6 test cases extracted from literature that accounted for different loading and unloading conditions as well as two different PCM materials (organic/inorganic) with different thermal properties. This constitutes a considerably wide validation range that supports model results and makes the model very promising for future energy analyses.

Fig.2 - Fig.7 show the validation results for each one of the 6 test cases consisting of the comparison of different model output variables and corresponding experimental values. Experimental data can be found in literature (Belmonte et al. 2016) in graphical format. Numerical values enabling computation of the proposed model were extracted using an open application for plot digitalization (WebPlotDigitalizer, 2018).

In order to ease the comprehension and interpretation of these results, the following legend should be taken into account:

- Figures A (upper left corner): Temperatures in ºC: Inlet fluid temperature (red), simulated outlet fluid temperature (green), real outlet fluid temperature (blue), ideal TES temperature (black)
- Figures B (upper right corner): Cooling power in kW: simulated value (green), real value (black)
- Figures C (lower left corner): Total cooling energy delivered along the test in kWh: simulated value (green), real value (black)
- Figures D (lower right corner): Percentage error in cooling energy delivered (blue)

It can be observed that, although outlet fluid temperature values do not match perfectly, the simulated values are able to capture quite satisfactorily the effect of the variable-temperature melting process revealed by the experimental measurements. As derived from Belmonte et al. (2016), this was not the case of the original approach, where the constant melting temperature showed clear deviations from real values.

In terms of outlet fluid temperature, the largest deviations are related to unloading tests (see Fig.4, Fig.5) probably due to the effect of subcooling phenomenon as well as of the non-linearity of the real h-T curves. These errors are still considered as acceptable, although they allow identifying potential aspects to focus on within future research and model improvements.

In addition, it can be stated that deviations in cooling power values are in line with those referred in the temperature analysis, and simulated cooling charge and discharge profiles are represented satisfactorily by the model.

Finally, in terms of cumulated energy transferred to the TES system, the aforementioned deviations are even reduced when computed along a relevant period of time (in this case 12-14h). Cooling energy charged or discharged during the tests is calculated by the model with a very narrow deviation from real measurements. Evaluating the phase change process, percentage deviations on the delivered energy are in any case lower than 10%.

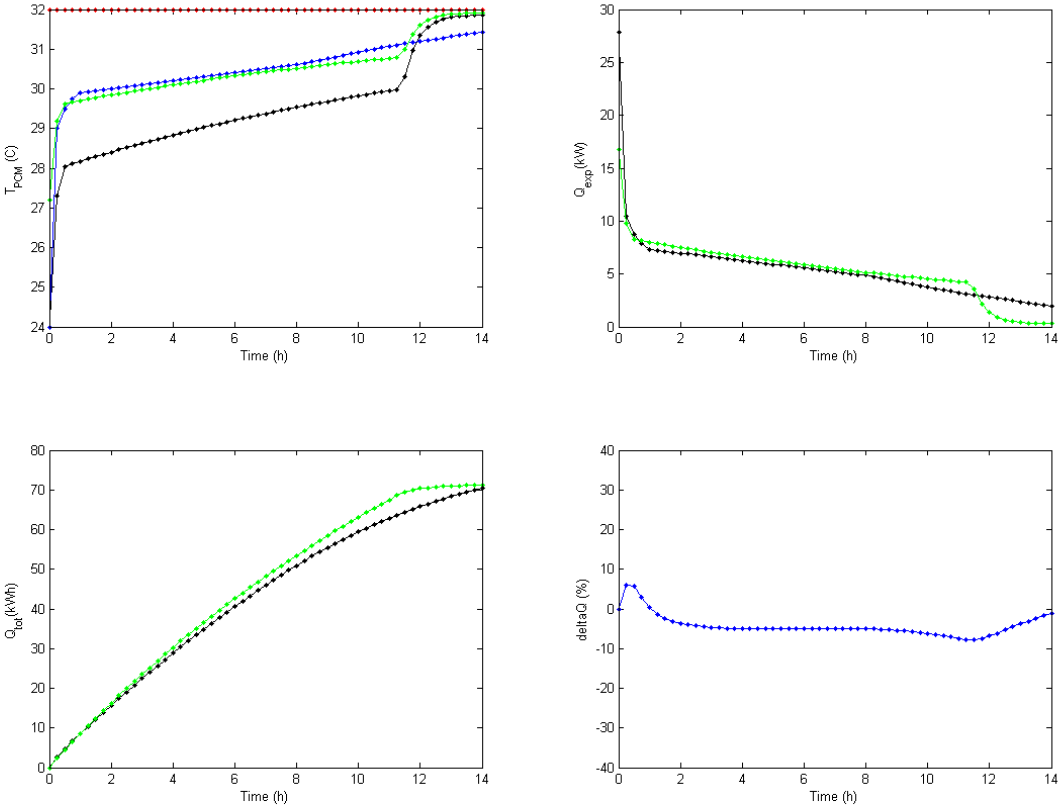

Fig.2: Comparison measured vs. simulated for the improved model validation: Inorganic PCM / loading test / initial temperature = 24 C / setpoint temperature = 32 C

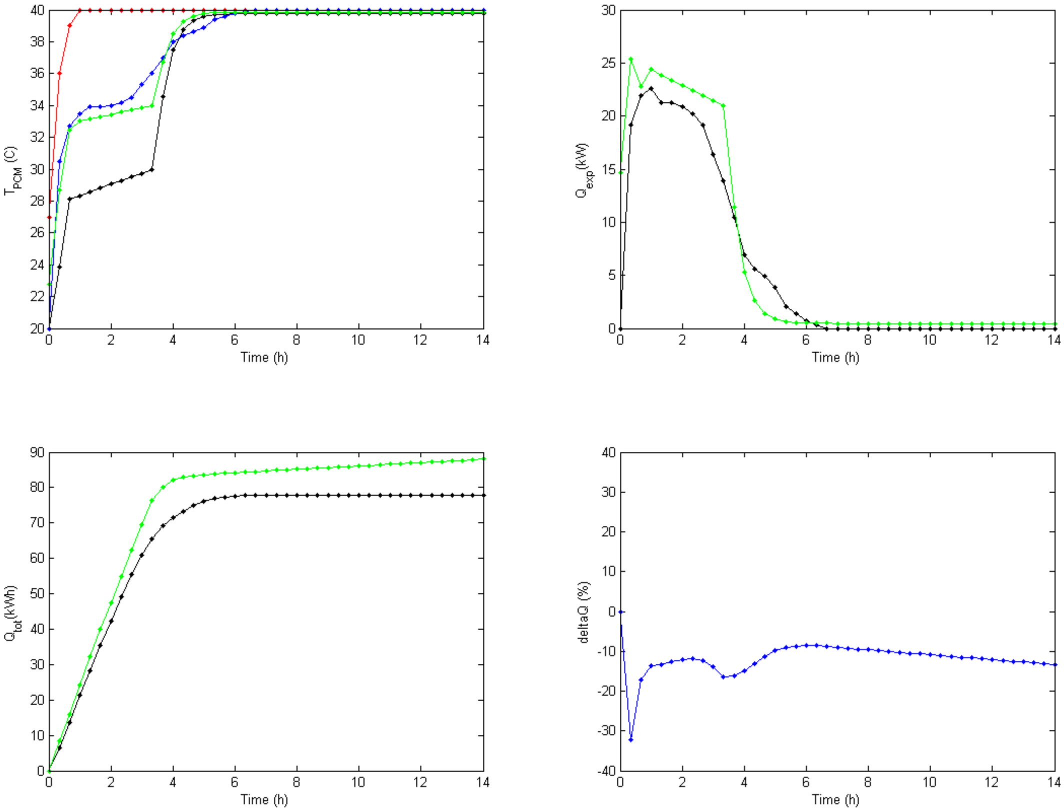

Fig.3: Comparison measured vs. simulated for the improved model validation: Inorganic PCM / loading test / initial temperature = 20 C / setpoint temperature = 40 C

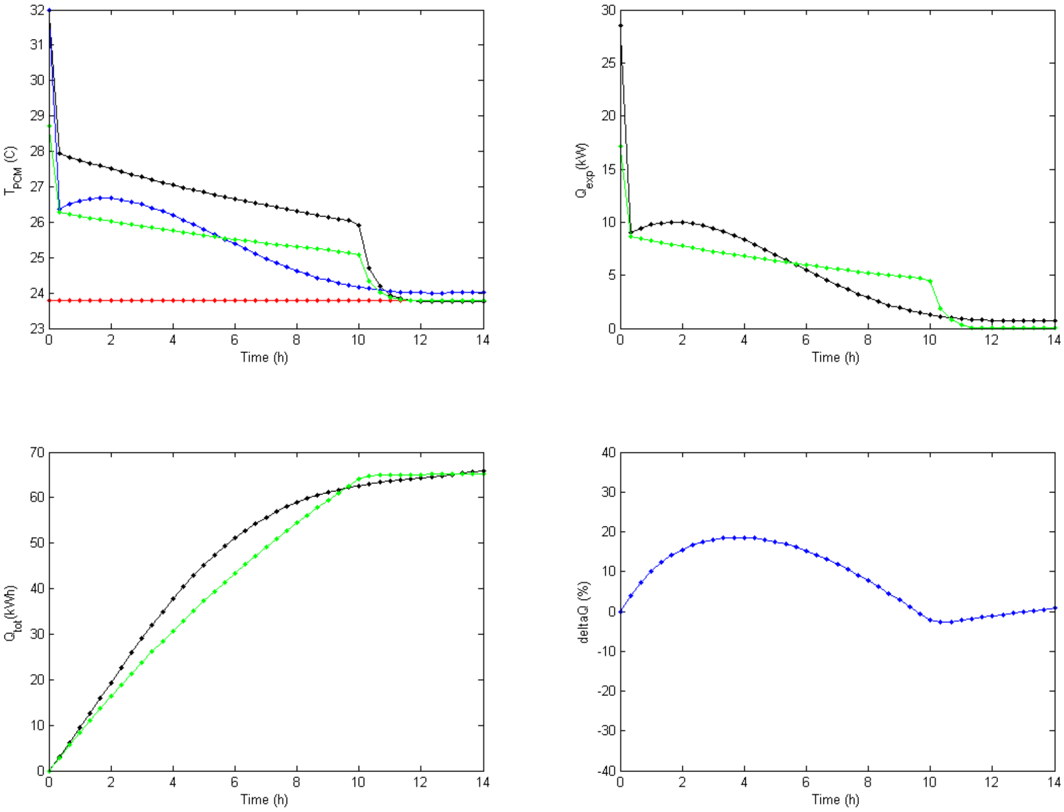

Fig.4: Comparison measured vs. simulated for the improved model validation: Inorganic PCM / unloading test / initial temperature = 32 C / setpoint temperature = 24 C

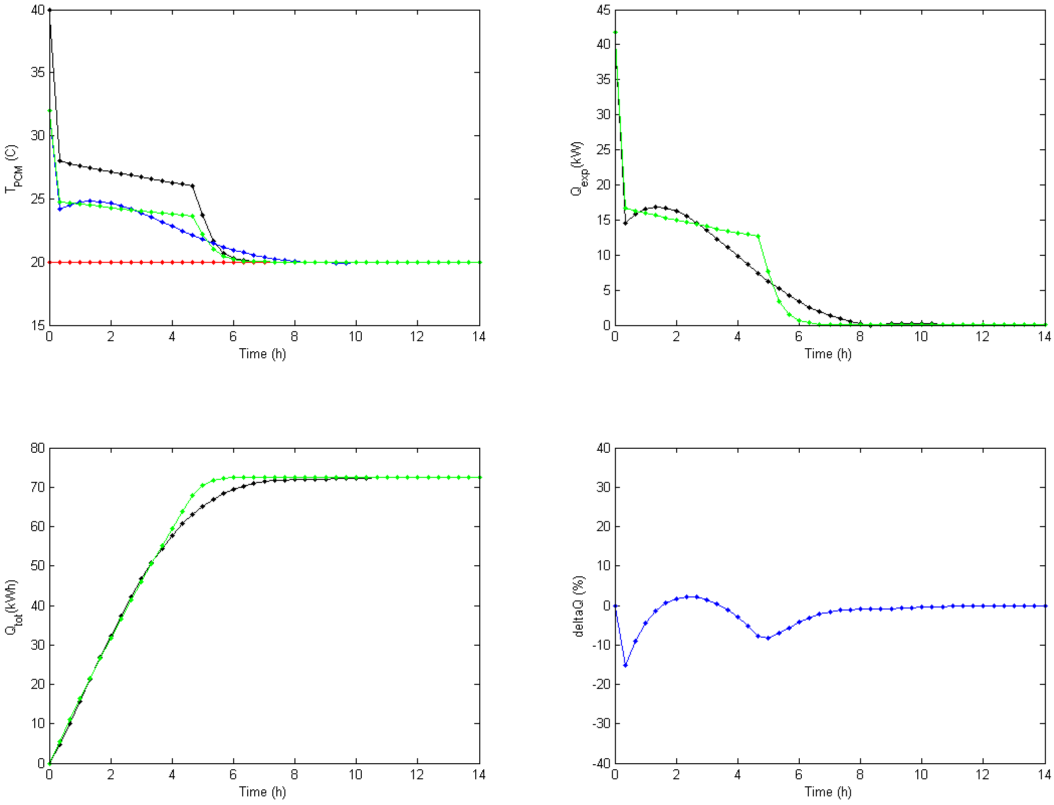

Fig.5: Comparison measured vs. simulated for the improved model validation: Inorganic PCM / unloading test / initial temperature = 40 C / setpoint temperature = 20 C

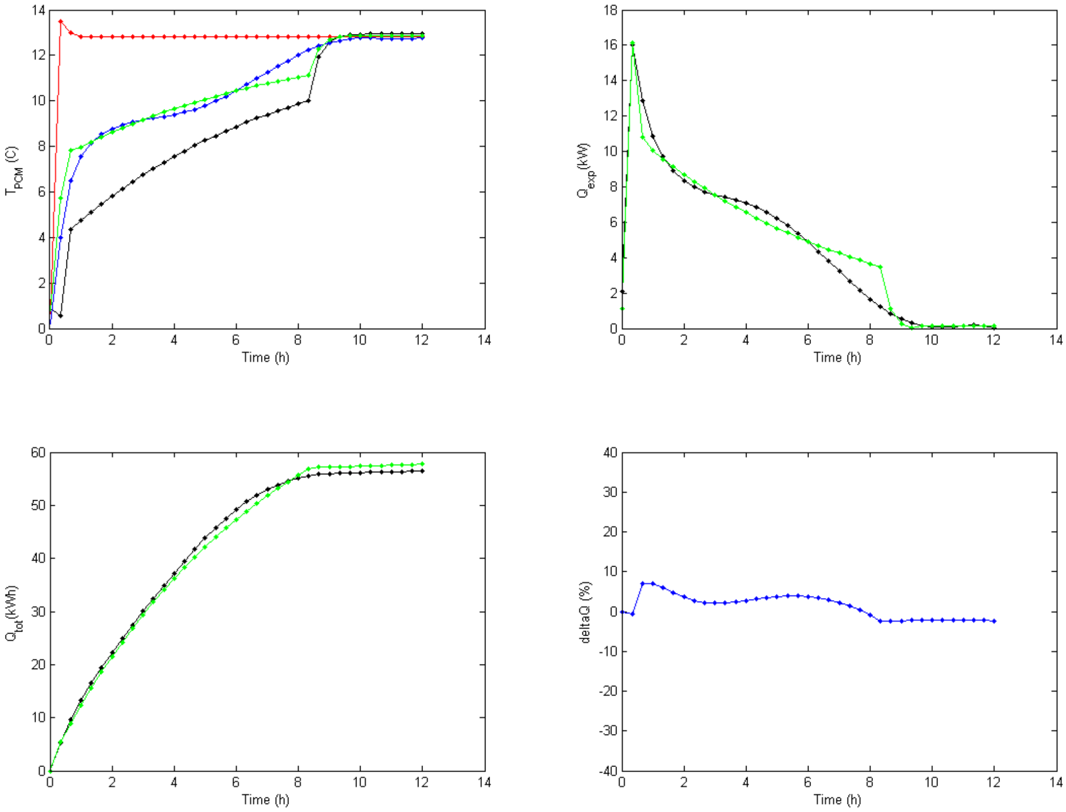

Fig.6: Comparison measured vs. simulated for the improved model validation: Organic PCM / loading test / initial temperature = 0.9 C / setpoint temperature = 13 C

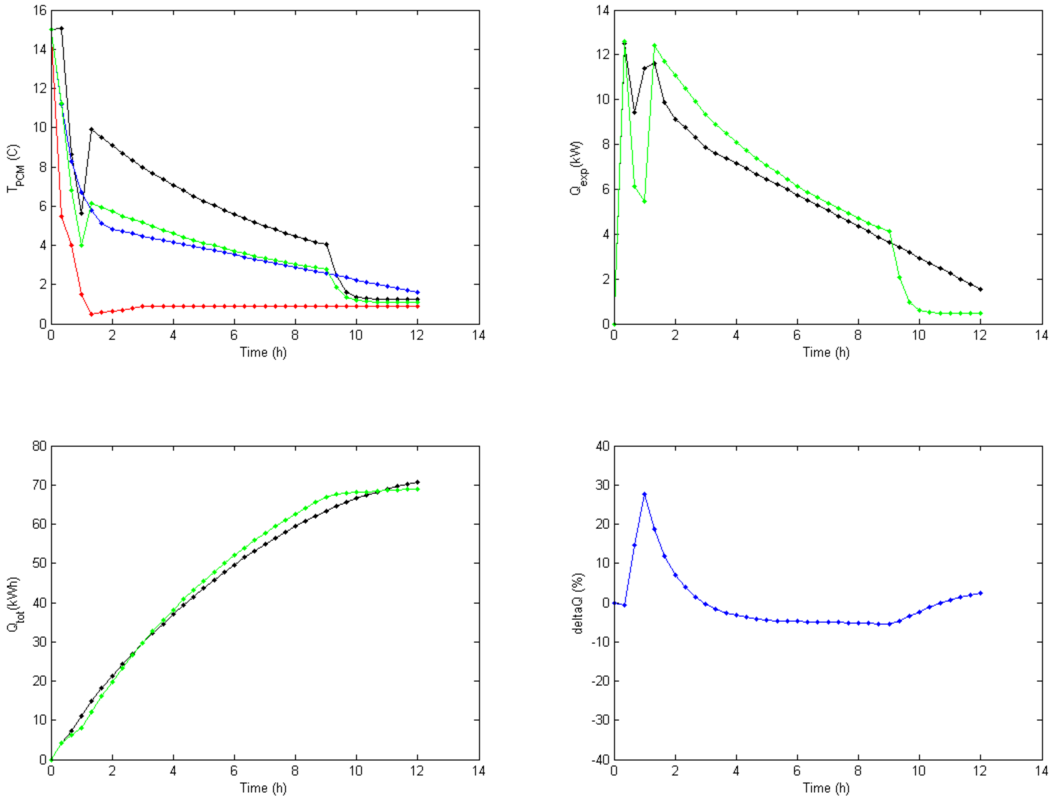

Fig.7: Comparison measured vs. simulated for the improved model validation: Organic PCM / unloading test / initial temperature = 15 C / setpoint temperature = 2 C

4. Conclusion

Comparison between experimental values and simulation results derived from the proposed PCM storage modelling approach proves highly satisfactory adjustment, being able to adequately capture the outlet fluid temperature profiles and leading to estimation errors lower than 10% in the cumulated energy transferred from/to the tank during the phase change process. Particularly, the improved representation of the PCM h-T curve reveals better behaviour than the original model presented in literature, while it does not add relevant complexity to the whole concept. This definition is only based on three very simple parameters that can be easily obtained from manufacturer PCM characterization, but provides noticeable improvements in outlet temperature and heat transfer estimations. The model has been implemented in MATLAB for validation, as well as embedded in a custom TRNSYS Type, so that it can be used in dynamic simulations to support design and analysis of sustainable energy concepts integrating PCM storage systems.

5. Acknowledgements

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