COMPARISON BETWEEN A NEW TRNSYS MODEL AND EXPERIMENTAL DATA OF PHASE CHANGE MATERIALS IN A SOLAR COMBISYSTEM

Jacques Bony, Stéphane Citherlet

Laboratory of Solar Energetics and Building Physics (LESBAT)
University of Applied Sciences Western Switzerland (HES-SO/HEIG-VD)
CH-1401 Yverdon-les-Bains – Switzerland

ABSTRACT

In the framework of the IEA Task 32 (Solar Heating and Cooling Programme), we developed a numeric model to simulate heat transfer in phase change materials (PCM), and experimental data. The analyzed system is bulk PCM plunged in a water tank storage of a solar combisystem (heating and domestic hot water production). The numerical model, based on the enthalpy approach, takes into account hysteresis and subcooling characteristic and also the conduction and the convection in the PCM. This model has been implemented in an existing TRNSYS type of water tank storage. The simulations has been compared with experimental data obtained with a solar installation using water tank storage of about 900 litres, already studied during the IEA Task 26 (Weiss 2003).

KEYWORDS

PCM, heat transfer, latent heat storage, solar energy, simulation.

INTRODUCTION

Thermal energy storage is an important topic for this new century. To increase the heat capacity of thermal storage, there are different possibilities. One of them is to use phase change material (PCM). Several studies have been already done using PCM module plunged in solar water tank storage (Egolf et al. 1997, Barba et al. 2003, Nagano et al. 2003, Plantier 2005, L. Cabeza et al. 2006, M. Ibanez et al. 2006, H. Schranzhofer et al. 2006, Nallusamy et al. 2007).

In the frame work of the International Energy Agency (IEA) Task32, focusing on advanced storage concepts for solar and low energy buildings (Hadorn 2005), different solutions are analysed such as PCM. On this topic, three groups have exchanged knowledge to developed different numerical models to simulate heat transfer in phase change materials (PCM) (Bony et al. 2005). On the other hand, different teams perform experimental test to evaluate PCM performance for thermal solar storage (Streicher 2007). Our group focuses on PCM modules plunged in a water tank storage, for which we have developed a numerical model and we have compared it with experimental measurements.

PCM/WATER STORAGE TANK MODEL

The numerical model had been implemented into an existing water tank model used in TRNSYS, called type60 (Klein S.A. et al). The existing model includes internal heat exchangers, 2 direct input-outputs and auxiliary heaters. The water tank can be considered vertically or horizontally. This model allows the simulation of most water storage tanks.

The number of horizontal segments called node or layer (Figure 1) determines the degree of calculation accuracy that can be improved with the increase of the node number. The initial maximum node number of 100 has been augmented up to 400. The height and the thermal losses of every layer can be defined separately. So it is possible to take into account the losses by a thermal bridge as for example a pipe junction.

\[
Q_{\text{medium}}^i = Q_{\text{flow}}(\text{in}) + Q_{\text{cond}}^i + Q_{\text{aux}} + Q_{\text{loss}}^i + Q_{\text{modules}}^i \quad (1)
\]

The energy exchange between the storage medium and the PCM modules is governed by the following equation (Bony et al. 2005):

\[
Q_{\text{modules}}^i = -N_{\text{modules}} \left( U_{\text{modules}} A_{\text{modules}}^i \left( T_i - T_{\text{PCM}}^i \left( h_{\text{PCM}}^i \right) \right) \right) \quad (2)
\]
The calculation of heat transfer through the PCM uses the enthalpy method (Visser 1986, Wang et al. 2003), which means, that for a given volume and material, a continuous and reversible function can be calculated, which will return the temperature \( T \) depending on the calculated enthalpy \( h \) shown in Figure 2. This enthalpy is used during the simulation to determine the node temperature at time \( t \).

\[ h(T) \]

\[ 
\begin{array}{c}
\text{Temperature} \\
\text{Enthalpy}
\end{array}
\]

\[ H_1 \quad H_2 \]

\[ 
\begin{array}{c}
\text{Solid} \\
\text{Phase change} \\
\text{Liquid}
\end{array}
\]

\[ T_1 \quad T_2 \]

**Figure 2** Example of an enthalpy curve for PCM.

The numerical model also takes into account the convection effect inside PCM, hysteresis and subcooling phenomena that can be observed with some phase change materials (Bony and Citherlet 2007).

The numerical resolution of the set of equations can be done by an explicit or implicit method. The explicit method is simple to program but is conditionally steady. It needs to have a time step smaller than a limit value. The implicit method is more complex to program but it is unconditionally steady. There is no limit for the time step except if we would like a good calculation accuracy.

We have chosen the explicit method, so it is necessary to pay attention to the time step in order to avoid a calculation divergence. The criteria of convergence are calculated with the following equations (Incropera 1990):

- for the interface water/PCM
  \[ Fo(2 + Bi) \leq 1/2 \] (3)
- for a node inside PCM material
  \[ Fo \leq 1/4 \] (4)
  \[ Fo = \frac{\alpha \cdot t}{\rho \cdot Cp \cdot x^2} \]
  \[ Bi = \frac{\alpha \cdot x}{\lambda} \]

From Equations (6) and (7), we get the maximum time step possible for calculation. It takes into account the heat transfer coefficients (convective and conductive) as well as the thermal capacity of every node and the position of the node considered (Incropera, 1990).

- for interface node water/PCM
  \[ t \leq \frac{\rho \cdot Cp \cdot x^2}{2\lambda(2 + \alpha \cdot x/\lambda)} \] (6)
- for a node inside material
  \[ t \leq \frac{\rho \cdot Cp \cdot x^2}{4\lambda} \] (7)

**PCM meshing**

The internal calculation model in the PCM is bi-dimensional, which allows the simulation of different PCM shapes: cylinder, sphere or plate. An onion peel approach has been used. It consists of representing a PCM element by a constant thickness layer succession whose shape depends on the object, as shown in Figure 3.

**Figure 3** Representation of the shapes available in the adapted TRNSYS model

For each node, we calculate the energy balance while supposing a uniform temperature in the volume of the corresponding node (Figure 4), which has an enthalpy variation given by the equation (8):

\[ \Delta h_{i,k} = \dot{Q}_{i,k-1} + \dot{Q}_{i,k} + \dot{Q}_{i+1,k} + \dot{Q}_{i,k+1} \]

Where the heat transfer at water-PCM interface (k=1) is:

\[ \dot{Q}_{i,\text{water}-\text{PCM}} = h_{i,\text{water}-\text{PCM}} \cdot A_{i,\text{water}} \cdot (T_{i,\text{water}} - T_{i,k}) \]

Where the heat transfer between 2 nodes of PCM is:

\[ \dot{Q}_{i,k-1} = \frac{\lambda_{\text{eff},i,k}}{x_{i,k}} + \frac{\lambda_{\text{eff},i,k-1}}{x_{i,k-1}} \cdot A_{i,k-1} \cdot (T_{i,k-1} - T_{i,k}) \]

**Figure 4** PCM mesh at the water-PCM interface and inside the material

In the Equation (10) the term of \( \lambda_{\text{eff}} \) is called effective thermal conductivity. It allows with a simple calculation to take into account the convection inside the PCM in the form of (Incropera, 1990, Cengel 1997):

\[ \lambda_{\text{eff}} = \lambda \cdot Nu \] (11)
Several equations exist to define convection inside cavities (Nusselt number). The cavity size, with its natural convection, influences the value of the convection coefficient. It would be necessary to take into account the height and the width of the cavity. However, some equations don’t use height notion for the convective cell, which simplifies its implementation in the code (Equations (12) and (13)). The validity range is for a ratio height/width between 1 and 40 for liquid. These values seem large enough to be used in a PCM module. Thus, we concentrated on the thickness determination of the liquid PCM layer to define the number of Nusselt in every node. Besides, during a thermal cycle, it is possible to have several liquid layers separated by a solid PCM layer.

The Nusselt number calculation is given by:

- Rectangular / cylindrical cavity: $10^6 < Ra < 10^9$ (Incropera 1990)

\[
Nu = 0.046Ra^{1/3} \quad [-]
\]  

(12)

- Spherical cavity: $10^2 < Ra < 10^9$ (Cengel 1997)

\[
Nu = 0.228Ra^{0.226} \quad [-]
\]  

(13)

To evaluate the conformity of the model, different experiments have been made with different PCM shapes like a cylinder or a sphere bed, and different PCM type like paraffin or sodium acetate trihydrate. We have made several comparisons with simulations and the numerical model gives a good result.

**EXPERIMENT**

Recently, we have experimented the performance improvement of a solar combisystem with PCM (Figure 5). This kind of installation provides thermal energy for domestic hot water (DHW) and heating demand for a building. This solar system has a water tank storage of 900 litres with 12 m² of a flat plate collector. There is an auxiliary gas burner integrated in the water tank (AGENA Energies).

**PCM choice**

Figure 6 shows the annual temperature frequency at four different heights in the water tank (only water). It has helped us to find the PCM to use according to the phase change temperature.

In the lower part of the tank, temperatures frequencies show a peak around 25 °C, whereas for the top of the tank the peak is around 60 °C.

For the experiment, 2 PCM type were selected. The first is sodium acetate with graphite (SGL Carbon) plunged in the upper part of the water tank. The second is paraffin RT27 (Rubitherm) in the lower part of the tank. The temperatures of phase change are respectively 58 and 27 °C. Different characteristics are given in Table 1.

**Table 1 PCM characteristics**

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Paraffin RT27</th>
<th>Sodium acetate graphite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity</td>
<td>0.2 (solid and liquid)</td>
<td>4 (solid and liquid)</td>
</tr>
<tr>
<td>Density [kg/l]</td>
<td>0.9 (solid) – 0.75 (liquid)</td>
<td>1.3 à 1.4 (solid and liquid)</td>
</tr>
<tr>
<td>Cp [kJ/kg]</td>
<td>1.8 (solid) – 2.4 (liquid)</td>
<td>2 (solid and liquid)</td>
</tr>
<tr>
<td>Latent heat [kJ/kg]</td>
<td>180</td>
<td>150</td>
</tr>
<tr>
<td>[kJ/l]</td>
<td>150</td>
<td>240</td>
</tr>
<tr>
<td>Phase change</td>
<td>27</td>
<td>58</td>
</tr>
<tr>
<td>temperature [°C]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure 5** Solar combisystem – thermal solar collector: 12 m², water tank storage: 900 liters

**Figure 6** Temperature frequency according to the height inside the water tank

**Figure 7** Sodium acetate with graphite (left) and paraffin RT27 (right)
PCM modules arrangement

The PCM is encapsulated in aluminium bottles, shown in Figure 8, before to place it in the water tank.

![Figure 8 Aluminum bottle and arrangement in the water tank](image)

The bottle size is:
- External diameter 88 [mm]
- Volume capacity 1.1 [l]
- Thickness wall 0.3 [mm]

A total number of 102 bottles have been installed, 60 of sodium acetate with graphite in the upper part of the tank and 42 of paraffin RT27 in the lower part (Figure 8). The PCM volume percentage is 21% in the top part and 14% in the bottom part. The global percentage is about 12%. This low value is due to the volume of the solar and DHW heat exchanger, and the combustion chamber through the middle of the storage tank.

Measurement

A test bench developed in our laboratory allows reproducing any weather condition and any building. Its working principle is based on successive physical measurements and numeric simulations on a minute timestep. The measures recorded by the LABVIEW program are written in a file which is read then by the TRNSYS program. TRNSYS simulates the weather, the solar sensors and the building behaviour. After simulation, TRNSYS writes a file of results which will be read by LABVIEW. It manages different devices to provide the right physical reaction to the solar installation. Figure 9 gives a preview of different parameters used during the tests and their physical or numeric source. The encircled part shows the solar combisystem.

![Figure 9 Diagram of different parameters measured or simulated in the test bench for solar combisystem](image)

The solar collectors are emulated by an electric heater whose power is controlled by the TRNSYS simulation according to the selected climate and collector type. The heating demand of the fictive building is achieved by a fan coil and a heat exchanger plugged on the cold water network. Solar gain and heating demand are controlled by PID. Domestic hot water draw off is managed according to a predefined time-table. The solar installation runs as if it is in a real house due to some temperature sensor emulated. These temperature sensors used by the controller are physically reproduced.

Test conditions

The test duration is 7 days with Zürich climate (Switzerland) which comes from the Meteonorm software (Meteotest). Figure 10 shows two different sequences of 7 representative days, selected for the comparison between simulation and experiment.

![Figure 10 Two 7-day climate sequences from Zürich. The first is a medium sunny winter and the second one is a high sunny winter.](image)
The emulated building is a well insulated single family house of 140m² floor area. The heat demand is 30 [kWh/(m².a)] (Weiss 2003). The energy per day for DHW is 7.5 [kWh]. During the 7 days, the total energy demand for heating and DHW is about 300 [kWh] for the first climate sequence and 200 [kWh] for the second.

RESULT AND DISCUSSION

Seven days test

We did some comparisons between measures and simulations in order to validate the water tank model with PCM. For example, the diagram of Figure 11 shows temperature differences in the storage tank without PCM between simulation and measures. This temperature comes from the upper part of the tank. The temperature increase shows when the burner is on. In this part of the water tank, the decrease of the temperature is due to the DHW draw off.

Figure 11 Temperatures in the upper part of the water tank without PCM (first climate sequence). Comparisons between the measures (full line) and the simulation (dotted line)

Figure 12 shows the same kind of diagram as figure 11 but with the PCM in the storage phase change material.

Figure 12 Temperatures in the upper part of the water tank with PCM (first climate sequence). Comparisons between the measures (full line) and the simulation (dotted line)

On these two figures, we can see that the numeric model is close to measurement. There are some differences, but the global behaviour during seven days is good.

Table 2 Gas energy comparison

<table>
<thead>
<tr>
<th>Value in [kWh]</th>
<th>Gas</th>
<th>Tank energy</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measurements</td>
<td>267</td>
<td>-4</td>
<td>263</td>
</tr>
<tr>
<td>Simulation</td>
<td>242</td>
<td>15</td>
<td>257</td>
</tr>
</tbody>
</table>

Figure 13 shows the result of comparison between measurement and simulation, for a solar combisystem with PCM, during 7 days of the first climate sequence. Figure 14 shows the same, but with the second climate sequence.

The differences in the energies are mainly due to the interactions between the different components, as the solar loop or the heating loop. Besides, the energy contained in the tank storage is bound directly to the burner on/off status just before the end of the test. Therefore, the sum of the gas consumption and the energy stored in the tank should be equal, as it can be seen in Figure 13. For instance in Table 2, we can see energy values:

Figure 13 Comparison measurement/simulation with PCM during 7 days (first climate).

Figure 14 Comparison measurement/simulation with PCM during 7 days (second climate).
DHW test

Figure 15 and Figure 16 show temperature in the upper part of the tank during a DHW test, respectively without and with PCM.

As we saw in Figure 11 and Figure 12, Figure 16 shows a very good fitting between the numerical model and measurement. We noticed after each burner startup or DHW draw off a heat transfer between water and PCM. After a big DHW draw off or an auxiliary startup it needs about 1 or 2 hours to get a complete heat exchange.

CONCLUSION

The developed numerical model allows achieving some simulations with PCM modules of different shapes (cylinders and vertical plates, beds of spheres) plugged in a water storage tank. This model, based on a representation in layer (onion skins), allows us to model the heat transfer evolution in the PCM, and between PCM and water. This model takes in consideration hysteresis, subcooling and PCM internal convection in liquid phase. The numerical model, included in an existing model of the TRNSYS software, has been compared with measures using different kinds of PCM (paraffin and hydrate salt) with cylindrical and spherical shapes (Egolf et al. 1996). The results showed a good correspondence between measures and simulations.

A comparison with a solar combisystem with or without PCM has been performed. Several 7-day measure tests, with different climates and DHW draw offs, have been tested. Simulations gave good enough results, in comparison with the experimental data, to go further on with annual simulation. These experimental results also allowed validating our numerical model. Thus it is enough reliable to perform other simulations without requiring data measurements. This model is also sufficiently adaptable to be used by any TRNSYS user.

On the other hand, we noticed an increase of the numbers of the burner starting when using the phase change material (Figure 11, Figure 12, Figure 15 and Figure 16). This increase of about 20 to 25% is due to the low heat transfer between water and PCM module. The heat exchange is not sufficiently fast to store auxiliary energy inside the phase change material modules. In our case, using PCM showed a behaviour going against all we expected. It would be necessary to increase the heat transfer between water and PCM. Several ways exist, for instance using smaller diameters of the PCM modules, which brings an increase of the surface/volume report. It would be also possible to add some small fins in the module with a high thermal conductivity.

This study showed also that it is difficult to improve the performances of this solar installation using PCM modules. At this time, it is difficult to conclude that phase change material doesn’t offer an advantage. In fact, the conception of this solar installation has been achieved without taking into account the PCM behaviour and the volume of the PCM modules that can be placed in the water tank is not very high (about 12%). Effectively, different internal heat exchangers are present inside the water tank. Furthermore, the heat transfer between water and PCM is not good with the diameter of the bottles used. The auxiliary power is too high compare to the heat transfer between water and the PCM modules.

With this new numerical model, it will be necessary to do complementary simulations to find a relation between the power to store energy and PCM characteristics. Then, it will be possible to define applications where it would be better to use phase change materials.

ACKNOWLEDGMENT

We would like to thank especially:

The Swiss Federal Office of Energy for financing this project.

Mr. Jean - Christophe Hadorn as the instigator of the IEA Task 32 for his support.
The IEA Task 32 participants for their collaboration and profitable exchanges.

The SGL Carbon Company for supplying sodium acetate with graphite which allowed us to achieve our study.

**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>$A$</td>
<td>exchange surface between 2 nodes</td>
</tr>
<tr>
<td>$A_{PCM}$</td>
<td>surface between water and PCM container.</td>
</tr>
<tr>
<td>$Bi$</td>
<td>Biot number [-]</td>
</tr>
<tr>
<td>$Cp$</td>
<td>PCM specific heat [J/(kg·K)]</td>
</tr>
<tr>
<td>$Fo$</td>
<td>Fourier number [-]</td>
</tr>
<tr>
<td>$h_{PCM}$</td>
<td>PCM enthalpy.</td>
</tr>
<tr>
<td>$i$</td>
<td>vertical axe (depend of number of water nodes)</td>
</tr>
<tr>
<td>$k$</td>
<td>horizontal axe (PCM meshing)</td>
</tr>
<tr>
<td>$N^{(modules)}$</td>
<td>number of PCM containers.</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number [-]</td>
</tr>
<tr>
<td>$Q^{(medium)}(i)$</td>
<td>energy of the storage medium of node $i$.</td>
</tr>
<tr>
<td>$Q^{(flow)}(i)$</td>
<td>charging or discharging energy via direct (inlet/outlet) flow including the flow upward and downward in the tank.</td>
</tr>
<tr>
<td>$Q^{(hxc)}(i)$</td>
<td>heat flux through internal heat exchanger.</td>
</tr>
<tr>
<td>$Q^{(aux)}(i)$</td>
<td>auxiliary energy.</td>
</tr>
<tr>
<td>$Q^{(cond)}(i)$</td>
<td>thermal conduction to neighbouring nodes.</td>
</tr>
<tr>
<td>$Q^{(loss)}(i)$</td>
<td>thermal losses through the tank envelope to the ambient.</td>
</tr>
<tr>
<td>$Q^{(modules)}(i)$</td>
<td>energy exchange between the storage medium and PCM modules.</td>
</tr>
<tr>
<td>$Ra$</td>
<td>Rayleigh number [-]</td>
</tr>
<tr>
<td>$t$</td>
<td>time step simulation [s]</td>
</tr>
<tr>
<td>$t_0$</td>
<td>initial time</td>
</tr>
<tr>
<td>$t_1$</td>
<td>final time</td>
</tr>
<tr>
<td>$T$</td>
<td>storage medium temperatures (node $i$).</td>
</tr>
<tr>
<td>$T^{(PCM)}$</td>
<td>surface temperature of PCM container.</td>
</tr>
<tr>
<td>$U$</td>
<td>heat transfer coefficient water/PCM.</td>
</tr>
<tr>
<td>$x$</td>
<td>distance between 2 nodes [m]</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>convective coefficient between water and PCM [W/(m²·K)]</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>PCM thermal conductivity [W/(m·K)]</td>
</tr>
<tr>
<td>$\lambda_{eff}$</td>
<td>effective thermal conductivity</td>
</tr>
<tr>
<td>$\rho$</td>
<td>PCM density [kg/m³]</td>
</tr>
</tbody>
</table>

**Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Meaning</th>
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<tbody>
<tr>
<td>PCM</td>
<td>Phase Change Material</td>
</tr>
<tr>
<td>DHW</td>
<td>Domestic Hot Water</td>
</tr>
<tr>
<td>PID</td>
<td>Proportional Integral Derivative</td>
</tr>
</tbody>
</table>

**REFERENCES**


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AGENA Energies, solar installation documentation.

SGL Carbon. Sodium acetate with graphite documentation.

Rubitherm. Paraffin documentation.

Meteotest. Meteonorm software to provide meteorological data.