EXTENSION OF A TRNSYS MODEL FOR LATENT HEAT STORAGE WITH PHASE CHANGE MATERIALS USED IN SOLAR WATER TANK

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1. INTRODUCTION

For several decades, different numerical models of storage tanks using PCM for latent energy storage have been developed; a few of these models have been elaborated to work with the TRNSYS simulation package (Jokisaalo, 2000). Unfortunately, none of them gave enough satisfaction to allow a large diffusion, either due to a lack of time to test its reliability (Visser, 1986), or a lack of flexibility which does not allow the modelling of different types of containers for PCM (Egolf, 1997).

In the framework of the IEA Task 32, which investigates advanced storage solutions in thermal solar systems for buildings, the potential of new PCMs is investigated to increase the energy density of small sized water storage tanks. This approach should have the advantage of reducing solar store volume for a given solar fraction as well as the store’s heat losses. It should also increase the solar fraction for a given available volume. To fulfill the Task’s requirements, we have developed a numerical model and compared data measurements with simulations results.

2. NUMERICAL MODEL

The developed model is an extension of the existing TRNSYS Type 60, for stratified fluid tanks based on sensible energy storage only (Klein, 2000). The tank can be made up to 100 fully mixed stacked volume segments (Figure 1a). This model has been adapted to be able to take into account the PCM calculation.

The standard Type60 includes internal heat exchangers, 2 direct input-output and auxiliary heaters. The water tank can be considered vertical or horizontal. This model allows the simulation of most of water storage tanks. The number of horizontal segments called also node (Figure 1a) determines the degree of calculation accuracy that can be improved with the increase of the node number. The height and the thermal losses of every layer can be defined separately. So it is possible to take into account the losses by thermal bridge as for example a pipe junction.

Figure 1b and equation (1) show the different heat fluxes of the energy balance considered in each $i^{th}$ node (segment or layer) of the water tank (Klein, 2000). For each node, the temperature is assumed to be uniform.
The energy balance for each storage node is given by the following equation:

\[ \dot{Q}_i^{(\text{medium})} = \dot{Q}_i^{(\text{flow})} + \dot{Q}_i^{(h)} + \dot{Q}_i^{(aux)} + \dot{Q}_i^{(cond)} + \dot{Q}_i^{(loss)} + \dot{Q}_i^{(modules)} \]  

(1)

With:
- \( \dot{Q}_i^{(\text{medium})} \) = energy of the storage medium of node \( i \)
- \( \dot{Q}_i^{(\text{flow})} \) = charging or discharging energy via direct (inlet/outlet) flow including the flow upward / downward in the tank
- \( \dot{Q}_i^{(h)} \) = heat flux through internal heat exchanger
- \( \dot{Q}_i^{(aux)} \) = auxiliary energy
- \( \dot{Q}_i^{(cond)} \) = thermal conduction to neighbouring nodes
- \( \dot{Q}_i^{(loss)} \) = thermal losses through the tank envelope to the ambient
- \( \dot{Q}_i^{(modules)} \) = energy exchange between the storage medium and PCM modules

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

\[ \dot{Q}_i^{(modules)} = -N_i^{(modules)} \left[ U_i A_i^{\text{PCM}} \cdot \left( T_i - T_{i,\text{PCM}}(k_i^{\text{PCM}}) \right) \right] \]  

(2)

With:
- \( N_i^{(modules)} \) = number of PCM containers
- \( U \) = heat transfer coefficient water/PCM
- \( A \) = surface between water and PCM container
- \( T \) = storage medium temperatures (node \( i \))
- \( T_{i,\text{PCM}} \) = surface temperatures of the PCM container

The calculation of heat transfer through the PCM uses the enthalpy method, which means that for a given volume and a 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 temperature is used during the simulation to determine the node temperature, according to the enthalpy of the system at time \( t \). Figure 2 shows this function constituted of a succession of 5 straight lines: two for the sensible heat in solid or liquid phase and three straight lines in the phase change part. Thus, the accuracy is enough for the calculations.
The numerical model also takes into account the hysteresis and subcooling phenomena that can be observed with some phase change materials. Although the developed model takes account of these two aspects, in the case of the studied paraffin here, these two phenomena are negligible. As it is out of the scope of this article, these phenomena are not detailed but will be published in another article.

**Numerical approach**

The numerical resolution of the set of equations can be done by an explicit or implicit method.

A) The explicit method is simple to program but is conditionally steady. It needs to have a time step smaller than a limit value in order to avoid any divergence. On the other hand it increases simulation time.

B) 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 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 a surface node: \( Fo(2 + Bi) \leq 1/2 \) (3)
- for a node inside material: \( Fo \leq 1/4 \) (4)

With:

\[
Fo = \frac{\lambda \cdot t}{\rho \cdot Cp \cdot x^2} \quad \text{et} \quad Bi = \frac{\alpha \cdot x}{\lambda}
\] (5)

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 different shapes available.

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

$$\frac{\Delta h^{i+1}_{i,k}}{\Delta t} = \dot{Q}^{i+1}_{i,k \rightarrow i-1,k} + \dot{Q}^{i+1}_{i,k \rightarrow i+1,k} + \dot{Q}^{i+1}_{i-1,k \rightarrow i,k} + \dot{Q}^{i+1}_{i+1,k \rightarrow i,k}$$

Where the heat transfer between 2 nodes is:

$$\dot{Q}^{i+1}_{i,k \rightarrow i-1,k} = \left( \frac{\lambda_{i,k} + \lambda_{i,k-1}}{x_{i,k}} \right) \cdot A_{i,k-1 \rightarrow i,k} \cdot \left( T_{i,k}^{i+1} - T_{i-1,k}^{i+1} \right)$$

With:
- \( i \) = vertical axe (depend on number of water nodes)
- \( k \) = horizontal axe (PCM meshing)
- \( \lambda \) = thermal conductivity
- \( x \) = distance between 2 nodes
- \( A \) = exchange surface between 2 nodes
- \( t_0 \) = initial time
- \( t_f \) = final time

The enthalpy at \( t_f \) time is

$$h^{i+1}_{i,j} = h^{i+1}_{i,j} + \Lambda h^{i+1}_{i,k}$$

Heat Transfer

The thermal conduction inside the PCM in the solid or liquid phase is the first phenomenon that we defined. In order to take into account the thermal conduction difference between the solid and liquid states of a material, the model allows 2 distinct values for the conduction coefficient; one for the solid and one for the liquid phase.

Figure 5 : Calculation of the thermal conductivity \( \lambda \) in accordance to the enthalpy H.
At the time of the phase change, the thermal conductivity value is calculated by linear interpolation of the enthalpy (Figure 5). Below the enthalpy value $H_1$, the thermal conductivity $\lambda$ is constant and equal to $\lambda_{sol}$. Above the enthalpy value $H_2$, the thermal conductivity is constant and is equal to $\lambda_{liq}$. Between $H_1$ and $H_2$, the conductivity is given by linear interpolation:

$$\lambda_{sol/lq} = \lambda_{sol} + \frac{(\lambda_{liq} - \lambda_{sol})}{(H_2 - H_1)}(H' - H_1) \quad (11)$$

Where, $H'$ is the enthalpy value at time step $t$ and given by eq. 10.

Then the convective coefficient between the water of the tank storage and the PCM container is calculated for every node and each time step, according to the container shape chosen:

- Plate and cylinder $\rightarrow$ vertical plate convection (Incropera, 1990)
- Sphere $\rightarrow$ convection around a sphere in free convection and in a sphere bed in forced convection (Achenbach, 1995).

Table 1 gives the different equations of the convective coefficient used according to the shape of the PCM module as well as the type of fluid flow around these modules (Incropera, 1990 and Achenbach, 1995).

Table 1 Equations for water / PCM convection.

<table>
<thead>
<tr>
<th>Convection</th>
<th>Vertical plate or cylinder</th>
<th>Sphere bed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laminar free</td>
<td>$Nu = \left{ \frac{0.825}{1 + (0.492/Pr)^{9/16}} \right}^{1/2}$</td>
<td>$Nu = 2 + 0.56 \left( \frac{Pr}{0.846 + Pr} \right)^{1/4}$ (Ra&lt;10^11)</td>
</tr>
<tr>
<td>Turbulent free</td>
<td>$Nu = 0.332 Re^{1/2} Pr^{1/3}$ (Re&lt;5.10^5)</td>
<td>$Nu_{laminar} = 0.664 \cdot (Re/\varepsilon)^{1/2} Pr^{1/3}$</td>
</tr>
<tr>
<td>Laminar Forced</td>
<td>$Nu_{laminar} = 0.664 \cdot (Re/\varepsilon)^{1/2} Pr^{1/3}$</td>
<td>$Nu_{turbulent} = \frac{0.037 (Re/\varepsilon)^{1/2} Pr}{1 + 2.443 (Re/\varepsilon)^{0.1} (Pr^{2/3} - 1)}$</td>
</tr>
<tr>
<td>Turbulent Forced</td>
<td>$Nu_{laminar} = 0.664 \cdot (Re/\varepsilon)^{1/2} Pr^{1/3}$ (5.10^5&lt;Re&lt;10^7)</td>
<td>$Nu_{global} = 2 + (Nu_{laminar}^2 + Nu_{turbulent}^2)^{1/2}$</td>
</tr>
</tbody>
</table>

Mixed Nusselt number and convective coefficient calculation with free and forced (water flow into tank storage) convection are given by (Incropera, 1990):

$$Nu_{Mixed} = (Nu_{free}^3 + Nu_{forced}^3)^{1/3} \quad (12)$$

$$\alpha = \frac{Nu_{Mixed} \cdot \lambda}{x} \quad \text{[W/m}^2\text{K]} \quad (13)$$

3. **EXPERIMENTAL DATA**

To validate the model, some temperature measurements have been performed. The temperature evolution inside the PCM during the charging and discharging cycle has been monitored with thermocouples placed inside a PCM module (paraffin). The time evolution of these temperatures has been compared with the simulation.

For these measurements, we have used an aluminium container whose diameter is 88 [mm], the height 150 [mm] and the thickness 0.3 [mm]. To keep a constant distance between the sensors, a grid and a cross in plastic have been used as shown in Figure 6a.
Then the liquid paraffin is poured in the container as shown in Figure 6b. The bottom part of the container remains open to allow sensor cables to be connected with the acquisition equipment. After the PCM has solidified, this container is plunged in the water tank with the sensor cables gone downwards. This method is possible because the liquid paraffin remains in the top of the container for the following reasons:

- The density of solid and liquid paraffin is lower than that of water
- The paraffin is non-miscible with water
- No high velocity of water flow inside the tank

**Measurements vs simulations**

A first step has consisted to compare the data measurements and the simulation results done with a model which did not take into account the convection inside PCM module. In this case, the temperature measurements done in the PCM module are very different to the results obtained by simulation, as the comparison between Figure 7 and Figure 8 shows. We can notice that the phase change is complete after 8 hours in this simulation instead of about 3.5 hours for the measurements.
Convection heat transfer

In order to improve the modelling of the heat transfer into the PCM module, we introduced an effective thermal conductivity which supports the convection in liquid phase of the PCM. It is given by:

$$
\lambda_{\text{effective}} = \lambda \cdot Nu
$$

(14)

Where, $Nu = $ Nusselt number for internal convection.

Two different equations describing the convection inside cavity have been compared manually (Incropera, 1990 and Cengel, 1997). As the results are similar, we have implemented the easiest equations in the model (equations (15) and (16)). These two equations don't use height notion for the convective cell, which simplifies its implementation in the code. Indeed, they require only the thickness of the PCM’s liquid layer to determine the Nusselt number at each node. Besides, during a thermal cycle, it is possible to have several liquid layers separated by a solid PCM layer.

The calculation of Nusselt number is given by:

- To a rectangular cavity with: $10^6 < Ra_L < 10^9$

  \[ Nu_L = 0.046Ra_L^{1/3} \quad [-] \quad (15) \]

  (Incropera, 1990)

- To a spherical cavity with: $10^2 < Ra < 10^9$

  \[ Nu = 0.228Ra^{0.226} \quad [-] \quad (16) \]

  (Cengel, 1997)

Figure 9: Measurements in laboratory (idem Figure 7)

Figure 10: Simulation taking into account internal convection inside PCM (20 nodes).

Figure 11: Simulation taking into account internal convection inside PCM (80 nodes).

Figure 10 shows results while taking into account the internal convection inside PCM. The small oscillations on the curves are generated by the non-continuity of the simulation model (meshing). It should be noticed that these oscillations have nothing to do with numerical instability. Between two spatial nodes, the change from solid to liquid is instantaneous for each layer depending on the temperature node. So, the effective conduction coefficient gets suddenly a strong variation between two time steps.

While increasing the node number for the PCM module calculations, it is possible to reduce the temperature oscillations as Figure 11 shows due to a reduction of spatial meshing.
On the other hand, simulation time increases also strongly with the increase of the node number. In the example of Figure 11, this simulation time is multiplied by a factor 30 for an increase of the calculation nodes of a factor 4 (20 to 80 nodes) as obtained in Figure 10. In future studies, requiring yearly simulations, it will be necessary to limit the node number in order to reduce calculation time.

4. CONCLUSION

The simulation of the heat transfer between water and PCM module is often difficult to solve. Indeed, the internal convection inside PCM module is often disregarded to simplify the model. This approach is only foreseeable for PCM having a very big viscosity. For the other PCM, such as paraffin, it is necessary to take into account the internal convection. The model presented here, uses the effective conduction coefficient approach.

The comparison between monitored data and the simulation model with convection results has shown a much better agreement compared to the simulation done by pure conduction (Figure 8). This method has an interesting potential and seems promising. However, it remains to confirm its qualities by performing other measurements and by reducing the temperature oscillations observed when the phase change occurs, without increasing significantly the simulation time.

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