# COMPARISON OF SYSTEM-LEVEL SIMULATION AND DETAILED MODELS FOR STORAGE TANKS WITH PHASE CHANGE MATERIALS

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## ABSTRACT

Numerical results of a new simplified model are compared to those of a detailed model for horizontal, liquid-based latent energy storage tanks filled with encapsulated PCMs of rectangular geometry. The simplified model is implemented as a TRNSYS component and the detailed model is built in COMSOL Multiphysics. Numerical results are compared to establish the consistency of the dynamic behaviour established from each model. Results indicate that the simplified model is capable of predicting the dynamic performance of this type of latent energy storage tank with reasonable accuracy in comparison to the detailed model. The validity of the assumptions made in the simplified model is confirmed. Some limitations associated with the use of such a model instead of a more physically accurate and computationally-intensive model are examined.

## INTRODUCTION

An obstacle to the use of phase change material in building energy systems is the lack of modelling tools available to HVAC system designers. Research in that area has led to many detailed, computation-intensive models which can trace the evolution in space and time of the solid-liquid interface within a volume. System-level performance simulation in buildings does not require such a level of detail, and reduced computing time is essential to perform long-term analyses and optimization studies.

Bony et Citherlet (2007) have modified a pre-existing stratified hot water storage tank model from TRNSYS, named Type 60, to include the effects of PCM capsules of various geometries. Model results for PCM filled cylinders in a vertical cylindrical storage tank agree quite well with experimental data once internal convection inside the PCM liquid phase is considered. The model uses a variable number of nodes over the PCM thickness and considers heat transfer between the adjacent PCM nodes which likely increases precision in emulating the phase change process but also increases computing time. The model allows some flexibility in defining the tank and PCM capsule geometry but limitations result from the choice of a convection correlation for vertical plates and inherent limitations in Type 60.

A 1-D model was produced by Liu and al (2011) based on Halawa's phase change processor (2010). The model represents the capsule geometry by a simple rectangle and does not consider any thermal resistance for the PCM material nor any heat transfer between adjacent PCM nodes. Experimental tests have determined there is a close agreement between the experimental and simulated outlet fluid temperature, though the model has some difficulties adequately representing experimental results at the beginning of the melting process.

As pointed out by Dutil et al. (2011), it is not advisable to use past studies to make general conclusions on what assumptions are reasonable in modelling PCMs. This paper compares the numerical results of a new simplified model to those of a detailed model for horizontal, liquid-based energy storage tanks filled with encapsulated PCMs of rectangular geometry.

## OBJECTIVES

The objectives of the study presented in this paper are to determine the validity of the assumptions made in the simplified model and to identify the limitations associated with the use of such a model instead of a more physically accurate and computationally-intensive model for building energy performance simulations that typically use system-level models to perform yearly or multi-year analyses. Significant changes were made to the model presented in D'Avignon & Kummert (2012) and the new model structure is presented. The paper then presents two studies that were performed with detailed COMSOL models to assess the validity of some assumptions made in the simplified model. Finally, the paper presents a comparison between the TRNSYS and COMSOL models and a discussion of the results.

## SIMPLIFIED MODEL

The simplified model will be used in full building performance simulations to test control strategies and establish accurate demand and/or energy savings related to the use of a latent energy storage tank. It is designed for maximum computability in annual simulations with small time steps (from 1 hour down to a few minutes) and aims to determine the latent heat storage tank outlet fluid temperature with sufficient accuracy, on the time scale of typical building system response.

The numerical model uses the control-volume based finite difference method referenced in Figure 1. The heat transfer fluid flows in the vertical space between two PCM capsules which is divided in a number of control volumes in the direction of flow. Each control volume encompasses only half the height of the fluid passage and similarly each PCM control volume is half the height of the PCM capsule. As conduction between adjacent PCM control volumes is neglected, the model is 1-D in the direction of flow; however each slice of the domain encompasses a fluid and a PCM control volume.

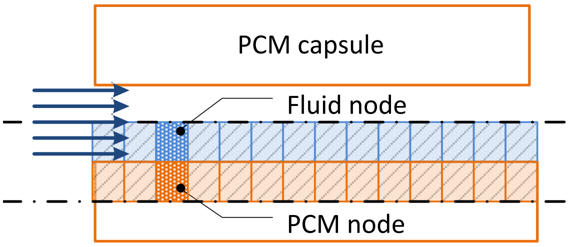


*Figure 1: Schematic of the modelled section of the latent energy storage tank in the 2D model*

The model is implemented as a TRNSYS component and is based on the following thermodynamic assumptions:

- Natural convection within the liquid phase of the PCM is neglected;
- No degradation or subcooling of the PCM is considered;
- Heat transfer occurs only through the upper and lower faces of the PCM capsules, lateral faces are considered adiabatic;
- Heat transfer between adjacent PCM control volumes is neglected.

Latent energy storage tanks function in three modes. First, the storage tank must be "charged" by melting or solidifying the PCM depending on whether heat or cold is to be stored. When the demand occurs, the tank's energy is then "discharged" as the PCM goes through the reverse change of phase. The third mode encompasses all that happens in between, that is during the period when the tank is not doing much but keeping the stored energy; the "waiting" mode. The first two modes function very much in the same way; forced convection between the capsule wall and the fluid is the predominant method of heat transfer. The "waiting" mode usually implies no fluid flow coming in or out of the latent energy storage tank and natural convection in the heat transfer fluid becoming important. In order to optimize the model's computability, separate mathematical formulations are used depending on the relative importance of advection and diffusion, using the thermal diffusion Peclet number, $Pe$, as a criteria.

### Important flow conditions | Pe > 100

For cases with high Peclet number, the fluid flow is important enough to force energy transfer between fluid nodes to occur mainly in the direction of flow. In this case, the influence of downstream conditions on the fluid temperature is low and space is considered a one-way coordinate (Patankar, 1941).

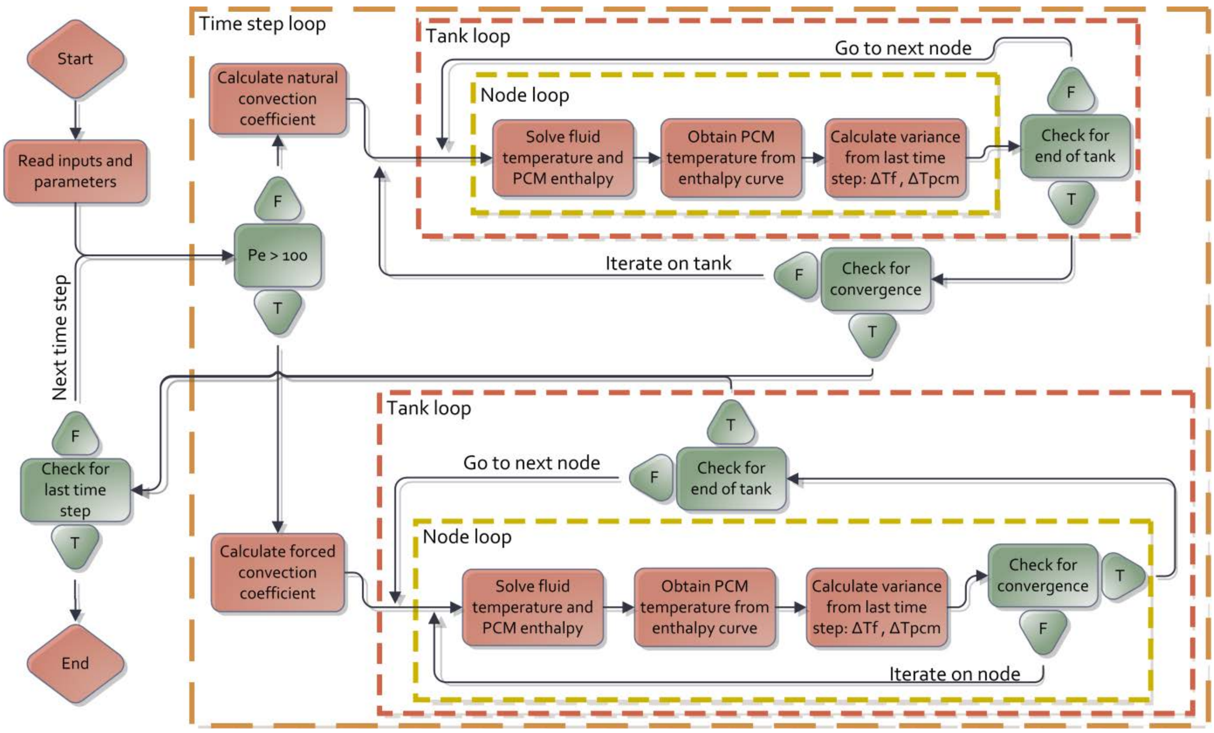


*Figure 2: Simulation flow chart*

As can be seen on Figure 2, a solution is obtained by marching in the direction of flow and solving for the fluid node temperature and its associated PCM node state to within the limits of the convergence criteria before moving on downstream to the next node. For each fluid control volume considered, the energy balance results in Equation 1:

$$\frac{\rho_f c_{p,f} V dT}{dt} = \dot{m} c_{p,f}(T_{in} - T_{out}) + h_{eq} A(T_{pcm} - T_f) \quad [1]$$

The term on the left represents the net rate of energy stored in the fluid control volume over a certain time step, with $\rho_f c_{p,f} V$ being the fluid's heat capacity. Term $\dot{m} c_{p,f}(T_{in} - T_{out})$ represents the net rate of energy transport into the control volume through advection. Term $h_{eq} A(T_{pcm} - T_f)$ represents the net rate of energy exchanged between the fluid and the PCM through convection, with $h_{eq}$ the equivalent heat transfer coefficient and $A$ the surface area of the heat exchange.

Using backward time differentiation to solve for Equation 1 would result in an implicit formulation that would offer some advantages regarding numerical stability. However, TRNSYS functions in such a way that the information passed along between components during an iteration are the time-averaged values over the time step concerned. Therefore it is more convenient to use time-averaged temperatures, $\bar{T}$, for the PCM and fluid which results in a semi-implicit scheme illustrated in Equation 2:

$$T_f = \frac{(a - b - c) * T_f^0 + b * \overline{T_{f(i-1)}} + c * \overline{T_{pcm}}}{a + b + c} \quad [2]$$

Here $T_f$ is the temperature of a given fluid node and similarly, $T_{pcm}$ is the temperature of a g iven PCM node. In this formulation, a= $\rho_f c_{p,f} V/\Delta t, b = \dot{m} c_{p,f}/2, c = h_{eq} A/2$, values from the previous time step are indicated with superscript "0" while values from the present time step bare no annotation. The upstream control volume is indicated with subscript "$(i-1)$" and the actual control volume bears no subscript.

The thermal mass of the capsule wall is neglected and an equivalent heat transfer coefficient, $h_{eq}$, is determined to account for all thermal resistances between the fluid and PCM, calculated in Equation 3.

$$\frac{1}{h_{eq}} = \frac{1}{h_c} + \frac{\Delta y/2}{k_{pcm}} \quad [3]$$

Where $h_c$ is the convective heat transfer coefficient, $\Delta y$ is the PCM node thickness and $k_{pcm}$ the PCM thermal conductivity. The convective heat transfer coefficient used, $h_c$, is the same for every node and is provided by Awad's correlation for a t hermally and hydraulically developing laminar flow between two plates at constant temperature (Awad, 2010). Term $(\Delta y/2)/k_{pcm}$ implies the conduction resistance between the capsule wall and PCM is evaluated over ½ of the PCM node height, to the center of the PCM control-volume.

To determine the fluid's impact on the PCM node, a variant of the so-called enthalpy method introduced by Voller (1990) is used where the temperature field in the PCM is not calculated explicitly but through enthalpy-temperature correlations. Thus the change in the PCM state is determined by calculating the change in enthalpy produced by the energy flux between the fluid and PCM nodes:

$$H = H^0 + h_{eq} A\{\overline{T_f} - \overline{T_{pcm}}\}\Delta t \quad [4]$$

Where $H$ is the current PCM enthalpy and $H^0$ is the PCM enthalpy for the same node from the last time step. The new PCM control volume temperature is then found through interpolation of the enthalpy-temperature curve.

At every time step, a stable solution is found for each control volume through the comparison of the different tank temperatures at the current and past time steps. The absolute change in temperature between two iterations must be less than $10^{-3}$ °C for the PCM temperature and HTF temperature for convergence to be reached. This method ensures a minimal number of iterations are required.

**Negligible flow conditions | Pe < 100**

For cases with low Peclet number, the heat transfer between the fluid and PCM nodes is considered to be caused solely by natural convection occurring in the fluid. Conduction between fluid nodes becomes an important heat transfer mode and so the fluid node heat balance becomes:

$$\frac{\rho_f c_{p,f} V dT}{dt} = \dot{m} c_{p,f}(T_{in} - T_{out}) + h_{eq} A(T_{pcm} - T_f) + \frac{k_f S}{\Delta x}(T_{f,(i-1)} - 2T_f + T_{f,(i+1)}) \quad [5]$$

Where S is the surface area perpendicular to the fluid passage, $k_f$ is the thermal conductivity and $\Delta x$ the length of the fluid node. Using backward time differentiation and time-average values over the time step for the PCM and fluid temperatures results in Equation 6, where $d = k_f S/\Delta x$. The convective heat transfer coefficient is provided by Globe and Dropkin's correlation for natural convection in a horizontal cavity (Incropera, Dewitt, Bergman, & Lavine, 2007).

$$T_f = \frac{1}{a + b + c + d}\left[(a - b - c - d)T_f^0 + (b + d)\overline{T_{f(i-1)}} + c\overline{T_{pcm}} + \left(\frac{1}{2}d\right)\overline{T_{f(i+1)}}\right] \quad [6]$$

Both the upstream and downstream fluid conditions will influence the fluid temperature and so a solution is obtained for every fluid node and its associated PCM node before verifying whether the convergence criterion is satisfied for every node of the entire tank. As can be seen on Figure 2, this method requires more iterations per time step than the marching-time procedure used in significant flow conditions and negatively affects calculation time.

## ASSUMPTION VERIFICATION: NO CONDUCTION BETWEEN PCM NODES

### Simulation

The first goal of this comparison exercise is to verify whether it is justified to assume there is no conduction between adjacent PCM nodes. In order to do so, a detailed model is built in COMSOL Multiphysics which allows easy modeling of additional thermodynamic phenomena; it is named the "2D" model. In this case, PCM capsules are modeled as a rectangular geometry and solely the part of the tank where the PCM capsules lay is modeled, hereby neglecting any impact from the restriction of the fluid coming into the space between the capsules. As can be seen on Figure 1, only the half height of the PCM capsule and half height on the passage between two capsules are modeled for increased computability (dashed area). Hence, the modeled geometry is exactly the same as the one assumed by the simplified TRNSYS model.

The detailed COMSOL model uses finite elements over the whole PCM and fluid domains so there are no "nodes" to speak of. Artificial nodes had to be created to allow a comparison to the nodal values calculated by the simplified TRNSYS model. These nodes are simple rectangles of the same width and height as those used in the simplified TRNSY model. They have only a geometrical representation in COMSOL; they are still composed of a finer finite-element meshing and are solved for concurrently. Integrating a v alue (temperature, for example) over the geometrical domain of an artificial node, provides a representation of the value calculated by COMSOL for that control volume and time step and can thus be compared to a nodal value from the same position and time step from the simplified TRNSY model. Whenever nodal values from the COMSOL models are discussed, it refers to the integrated value over the artificial node geometry.

*Table 1: Material characteristics*

| FLUID PROPERTIES | VALUE | UNITS |
|---|---|---|
| Specific heat | 4182 | J/kg-°C |
| Density | 989.9 | kg/m$^3$ |
| Thermal conductivity | 0.62556 | W/m-°C |
| Dynamic viscosity | 5.86*10$^{-4}$ | Pa*s |
| **PCM PROPERTIES** | **VALUE** | **UNITS** |
| Specific heat capacity | 2410 | J/kg-°C |
| Volumetric heat capacity | 333 | MJ/m$^3$ |
| Density | 1587 | kg/m$^3$ |
| Thermal conductivity | 0.450 | W/m-°C |
| Latent heat of fusion | 210 000 | J/kg |
| Melting temperature | 46.1 | °C |
| Freezing temperature | 45.9 | °C |
| Initial temperature | 30.0 | °C |

A flat velocity profile condition is imposed to the fluid coming into the vertical space between two capsules. The evolution of the fluid flow profile throughout the length of the PCM capsule is determined through the use of the continuity equation and the heat equation.

The simulation created uses water as the heat transfer fluid with thermal properties held constant at the values found in Table 1. The phase change material used is PCM Products's salt hydrate S46 which is said to have the same thermal properties for both its phases (PCM Products Ltd, 2009). The PCM capsule modeled is 0.5 m long, 0.25 m wide and 0.038 m in height, with a spacing of 0.013 m between two capsules to allow fluid passage.

Two test cases (see Table 2) are created to account for a v ariety of circumstances combining either of two different flow speeds at the entrance of the fluid passage. As properties are the same for the liquid and solid phases of the PCM, a cooling process with the PCM remaining in its liquid phase and a heating process of the PCM remaining in its solid phase give the same results and so only heating cases are discussed here. All simulations were run for 3000s.

*Table 2: Data for simulation test cases*

| TEST CASE 1 : HEATING, LOW FLUID SPEED | |
|---|---|
| Initial fluid and PCM temperature | 30 °C |
| Incoming fluid temperature | 45 °C |
| Low fluid speed | 0.01 m/s |
| **TEST CASE 2 : HEATING, HIGH FLUID SPEED** | |
| Initial fluid and PCM temperature | 30 °C |
| Incoming fluid temperature | 45 °C |
| High fluid speed | 0.05 m/s |

The detailed COMSOL model uses PCM nodes tightly squeezed against each other and the conductivity of the PCM itself applied at the interface between two nodes. This detailed COMSOL model is compared to an alternative version where a thin thermally resistive layer (TTRL) of 1 mm in depth and a thermal conductivity of 1*10$^{-6}$ W/m-K is inserted between PCM nodes.

### Results and discussion

The ratio of the energy flowing to and from adjacent PCM nodes to the total energy entering or leaving a PCM node is evaluated for each simulation test case. It is found that heat transfer with adjacent PCM nodes becomes increasingly important as time passes, its contribution peaking at 6.76% of the total energy transferred to/from the PCM node for test case 1. However, the highest energy fluxes between PCM nodes occur at the beginning of the simulation, specifically at the first moment the entering fluid temperature front reaches each fluid node. Hence, as illustrated on Figure 3, the moment the contribution of the heat transfer with adjacent PCM nodes becomes significant in proportion; its absolute values are excessively small. The highest ratios are associated with the first PCM nodes encountered in the direction of flow, which is coherent with the fact that these nodes are subjected to hotter fluid temperatures and thus higher temperature gradients between adjoining fluid and PCM nodes.

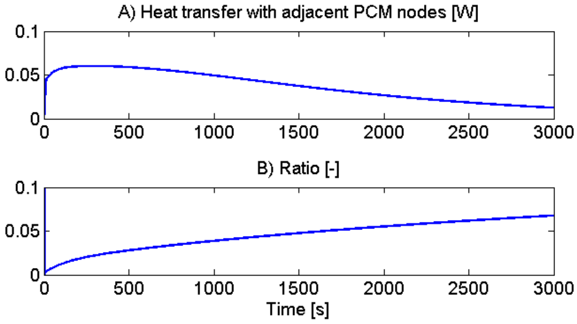


*Figure 3: Results for the 2nd PCM node in test case 1*

Comparing the evolution of the outlet fluid temperature through time for both models (2D model with and without the TTRL) in all test cases yields nearly identical results; the maximum absolute difference between the two datasets being less than 0.017 degrees Celsius. Thus, though heat transfer between adjacent PCM nodes is undeniably present, neglecting its contribution remains justifiable for the simplified TRNSYS model as its impact on the evolution of the output fluid temperature is negligible.

## ASSUMPTION VERIFICATION: NON-DEVELOPED VELOCITY PROFILE AND SIMPLIFIED GEOMETRY

### Simulation

In the simplified TRNSYS model, the fluid speed used in calculating the Reynolds number and later the Nusselt number and heat transfer coefficient $h_c$ is obtained from the fluid mass flow rate entering the tank assuming a uniform fluid velocity profile across the height of the fluid passage. The impact of this assumption is evaluated by comparing the results from three COMSOL models. The 2D model described previously imposes a null fluid velocity condition at the capsule wall, forcing the fluid flow to develop into a boundary layer following the continuity equation and the Navier-Stokes equation. The "slip" model is a duplicate of the 2D model but the boundary condition at the capsule wall is modified to force fluid flow to "slip" along the capsule face, thus keeping the fluid velocity profile undeveloped over the length of the capsule. Lastly, a 3D model is created that has the same null fluid velocity condition at the capsule surface as the 2D model but also considers the impact of the real capsule geometry on the flow velocity profile.

The simplified TRNSYS model uses a simple rectangle to represent the PCM capsule geometry. As can be seen on Figure 4, the capsule's top and bottom surfaces are in fact covered with a series of empty protrusions that fit together to hold the capsules at a specific distance away from one another. The top and bottom surfaces have a series of holes which penetrate to the capsule center. The capsule's downstream lateral face also includes a depression where the sealed filling orifice is located, but this geometrical feature is not considered here. The realistic geometry increases the PCM volume by only 0.025% compared to the 2D model but increases the heat transfer surface by 3.9 %. Thermohydraulic simulations of Case 1 described previously allowed to evaluate the fluid velocity as it circulates in the space between two PCM capsules.

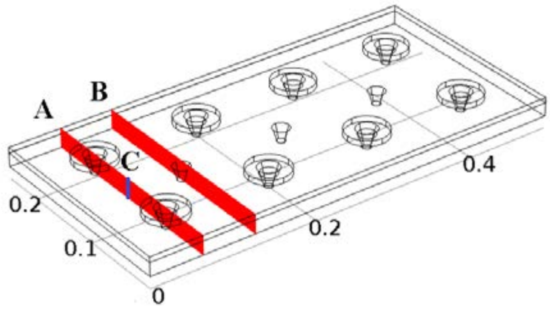


*Figure 4: Capsule geometry of 3D model*

### Results and discussion

Results from the 2D model indicate the fluid forms a fully developed profile which reaches speeds of up to 0.0149 m/s. The flow profile evolves rapidly becoming fully developed in less than 40 s, at a distance of 0.2 m from the leading edge of the PCM capsule. In the case of the slip model, the flow profile remains constant along the height of the fluid passage and along the length of the PCM capsule at a value of 0.01 m/s.

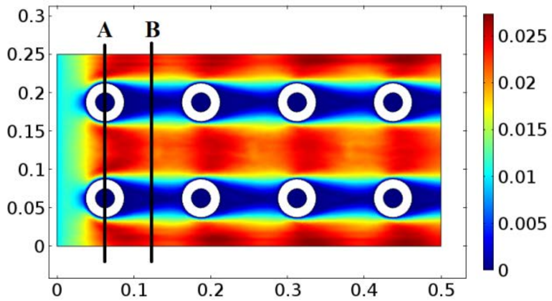


*Figure 5: Velocity profile [m/s] at the half-height of the fluid passage for the 3D model*

For the 3D model, Figure 5 illustrates the velocity profile of the heat transfer fluid along the half-height of the fluid passage at t=1500 s. In the sections behind the protrusions, flow velocity tends towards zero. Where no protrusions interfere, the flow velocity is much higher than the 0.01 m/s imposed in the simplified TRNSYS model, reaching velocities as high as 0.0275 m/s.

The capsule geometry also has important impact on the heat transfer into the PCM and is analyzed at specific sectional views. As shown on Figure 4, Section A intersects the protrusions perpendicular to the direction of fluid flow and Section B cuts through the first hole along the capsule's centerline. Thermal analysis of Section A for t=1500 s, shown in Figure 6, indicates the protrusions act as thermal barriers, impeding heat transfer to the PCM below and the same can be said of the fluid trapped inside those protrusions. Though the holes along the capsule center see little flow, Section B indicates they act like thermal bridges to the center of the capsule. Zones in Figure 5 where the fluid speed is highest are also those where the PCM temperature is highest in Figure 6, indicating the higher flow velocities have locally increased heat transfer to the PCM capsule.

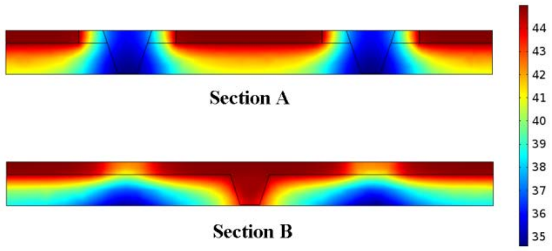


*Figure 6: Temperature distribution inside the PCM capsule after 1500 seconds*

The temperature distribution visible on sectional cuts from Figure 6 indicates a significant temperature gradient over the half height of the PCM capsule. Even greater temperature gradients occur over the half height of the PCM capsule near the beginning of the simulation. A vertical line C cutting through the PCM is located at half the width of the capsule and one eighth of the way along the capsule length, as illustrated in blue on Figure 4. The temperature gradient evaluated along line C is presented for various time steps on Figure 7.

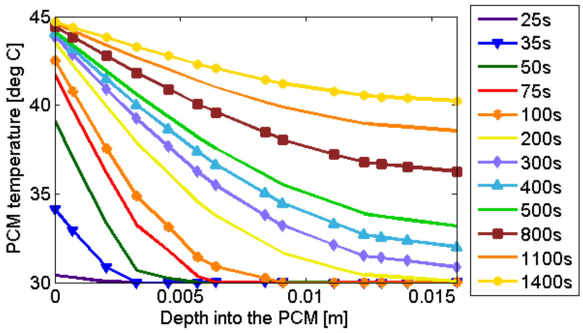


*Figure 7: Temperature gradient over line C*

For t=75s to t=500s, the temperature gradient along the height of the PCM is greater than 10°C, reaching a variation of as much as 13.4 °C at t=200s. The simplified model assumes one node along the depth of the PCM slab, i.e. a uniform temperature in the curves shown in Figure 7. The strong temperature gradients shown in the COMSOL results show that this assumption could cause significant errors in the instantaneous heat transfer between each PCM and fluid nodes. The temperature also varies along the width of the PCM capsule but only in the areas surrounding the protrusions and holes. In the TRNSYS model, these protrusions and holes are replaced by an equivalent horizontal surface so the use of a single node over the width of the PCM capsule should be adequate.

The evolution of the outlet fluid temperature through time for test Case 1 is presented in Figure 8 for all three models. A significant difference between the 2D and Slip models occurs at the beginning of the simulation when a difference of over 1°C is shown between t=36s and t=56s, reaching a maximum value of 7.03 °C. However, the mean absolute difference between these two simulations is only 0.53 °C over the length of the whole simulation. The fluid flow profile appears to have significant impact on the outlet fluid temperature only for the few time steps surrounding the moment when the hot fluid entering the tank first reaches the tank's outlet.

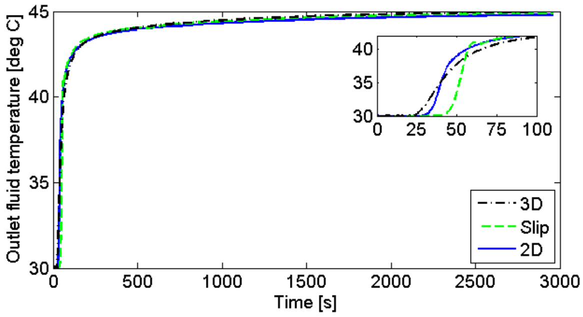


*Figure 8: Outlet fluid temperature for Case 1*

The differences between the models are most significant at the beginning of the simulation (between t=25s and t=75s). The moment when the outlet fluid temperature begins to increase above 30°C and the speed with which it stabilizes at about 44°C is different for all three models. The onset of the outlet fluid temperature heating up occurs faster for the 2D and 3D models due to the fact that the developed flow profile allows higher fluid speeds over parts of the passage between two capsules, some hot inlet water thus reaching the end of the capsule faster than in the Slip model. The increase of outlet fluid temperature is centered at 50s for the Slip model, which is consistent with the 0.01 m/s fluid velocity. In the case of the 2D model, the increase in outlet fluid temperature is centered around 30 to 35s.

Though the real capsule geometry's impact on the flow and temperature distribution is evident on Figure 5 and Figure 6, the maximum absolute difference between results from the 2D and 3D models is only 1.95°C. The mean absolute difference between these two models is only 0.34°C, concluding the real capsule geometry is reasonably well represented by the simple rectangle used in the 2D COMSOL model and simple TRNSYS model. The 3D model has the most slanted profile, likely caused by the enhanced heat transfer from the fluid to the PCM due to an augmented capsule surface and increased fluid speeds. Future experimental results will confirm whether this behaviour is observed in practice and whether the simplified model needs to be adapted to take these effects into account.

## MODEL COMPARISON

### Simulation

An important goal of this comparison exercise is to verify whether the simplified model represents the phase change process in a reasonable manner. In order to do so, the 2D detailed model built in COMSOL Multiphysics is modified to account for phase change in the capsule material. Porous media physics are used to model the PCM as a solid porous matrix with a liquid media flowing through it. The time-varying proportion of the fluid to the porous matrix (a.k.a the liquid fraction) is controlled by the evolution of the domain's enthalpy along the enthalpy-temperature curve, as it is done in the simplified TRNSYS model. The heat equation and continuity equation control the heat flow as in the previous models. The PCM properties used are those of Table 1.

*Table 3: Phase change test case detail*

| | |
|---|---|
| **MODE 1 : HEATING** | |
| Initial fluid and PCM temperature | 30 °C |
| Incoming fluid temperature | 62 °C |
| Low fluid speed | 0.01 m/s |
| Duration | 4 950s |
| **MODE 2 : WAITING** | |
| Incoming fluid temperature | 45 °C |
| No incoming nor outgoing fluid | 0 m/s |
| Duration | 4 950s |
| **MODE 3 : COOLING** | |
| Incoming fluid temperature | 30 °C |
| Low fluid speed | 0.01 m/s |
| Duration | 4 950s |

A test case is formulated including all three modes of typical energy storage; each mode is described in Table 3 above. As neither the simplified TRNSYS model nor the 2D COMSOL model as of yet include any losses to the tank's surrounding environment, the second mode ("the waiting mode") allows the PCM tank temperature to even out but the total energy within the tank remains constant.

### Results and discussion

For HVAC systems designers, the most significant information acquired from the numerical model of a latent energy storage tank is the energy exiting the tank. As the fluid flow is imposed by the rest of the system and not modified by the storage tank, the temperature of the fluid exiting the tank is the significant variable the model needs to be able to simulate adequately and is illustrated in section A) of Figure 10 for both models. Note that during the "waiting mode" (from t=4950s to t=9900s), there is no fluid flow and so the "outlet fluid temperature" does not exist. The temperature of the last fluid node is represented in the Figure for these periods (highlighted by a grey background.

Results indicate the main differences occur closely after the onset of a large change in inlet fluid temperature or velocity; close-ups can be seen in Figure 9 at both moments when such changes occur in the test case. However, both curves are centered at 50s in the heating mode and at 9950s for the cooling mode. The COMSOL models stabilizes at a much lower temperature than the TRNSYS model in the heating mode and at a higher temperature in the cooling mode indicating increased heat transfer from the fluid to the PCM.

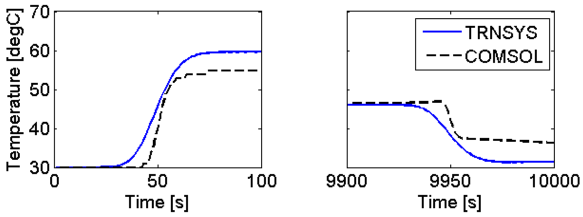


*Figure 9: Close-up of outlet fluid temperature for the simplified TRNSYS model and 2D COMSOL model*

As the second mode tested involves no outgoing fluid flow, the significant outputs studied from both models cannot be limited to the outlet fluid temperature. Therefore, the PCM liquid fraction and the average PCM temperature are also compared in sections B) and C) of Figure 10.

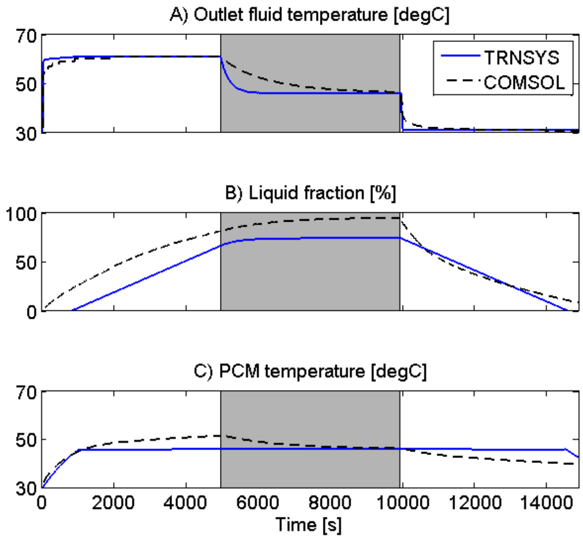


*Figure 10: Results from the simplified TRNSYS model and 2D COMSOL model*

The evolution of the liquid fraction through time confirms the different outlet temperature profiles are caused by greater heat transfer to the PCM in the COMSOL model. As natural convection in the fluid is neglected in the simplified model when $Pe > 100$, the reduced heat transfer coefficient could be the cause of the lessened heat transfer between the fluid and PCM. Agyenim et al. (2010) claims models based on either pure conduction or pure convection within the PCM have not been able to predict accurately the melting rates in either the solid or liquid phase of the PCM. Though Zivkovic and Fujii (2001) concluded natural convection in the PCM's liquid phase could be neglected for long, thin capsules, this deficiency in the simplified model could also explain part of the reduced heat transfer in comparison to the detailed model.

It is also apparent that finite-volume modelling restricts the variation of temperature in the PCM as the whole volume of each PCM node in the simplified model is considered to be at the same temperature. The effect would be attenuated were there to be more nodes over the half height of the PCM capsule. The effect of the more detailed modelling can also be seen in the calculation time. Where the COMSOL model requires 4 hours and 24mins to compute the test case results, the TRNSYS model requires only 7.5s.

## DISCUSSION AND CONCLUSION

A simple model simulating the transient behaviour of a latent energy storage tank with rectangular PCM capsules is developed in TRNSYS. Following the analysis of the results obtained by detailed COMSOL models, it is concluded that neglecting conduction between adjacent PCM nodes does not introduce a significant error in the prediction of the outlet fluid temperature and that the capsule geometry can be adequately represented by a simple rectangle. The use of a single PCM node over the half-height of the capsule introduces significant errors after a s harp transition in the incoming fluid speed or temperature, so additional PCM nodes will have to be included. The experimental validation phase of our work will help fine-tuning the positioning of these nodes and the choice of convection coefficient correlations. The level of accuracy and the computational effort associated with the developed TRNSYS component are in line with the objective of obtaining a model suitable for system-level analyses.

## NOMENCLATURE

A = surface area, PCM to fluid node [$m^2$]
$c_p$ = constant pressure specific heat [J/kg*K]
H = enthalpy [J]
h = heat transfer coefficient [W/K-$m^2$]
k = thermal conductivity [W/m-K]
$\dot{m}$ = heat transfer fluid mass flow rate [kg/s]
Pe = Peclet number [-]
T = temperature [K]
$\bar{T}$ = time-averaged temperature [K]
S = surface area between fluid nodes [$m^2$]
V = volume [$m^3$]

**Greek symbols**

ρ = density [kg/$m^3$]
$\Delta t$ = simulation time step [s]
$\Delta x$ = length of fluid and PCM nodes in the direction of flow [m]
$\Delta y$ = height of PCM node [m]

**Subscript**

c = convective
eq = equivalent
i-1 = values from the upstream control volume
i+1 = values from the downstream control volume
in = incoming
f = heat transfer fluid
l = liquid state
out = outgoing
pcm = phase change material
s = solid state

**Superscript**

0 = values from the previous time step

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