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Simplified Numerical Description of Latent Storage Characteristics for Phase Change Wallboard

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ABSTRACT

Cooling of residential California buildings contributes significantly to electrical consumption and peak power demand. Thermal mass can be utilized to reduce the peak-power demand, down-size the cooling systems and/or switch to low-energy cooling sources.

Large thermal storage devices have been used in the past to overcome the short-comings of alternative cooling sources or to avoid high demand charges. With the advent of phase change material (PCM) implemented in gypsum board, plaster or other wall-covering material, thermal storage can be part of the building structure even for light-weight buildings. PCMs have two important advantages as storage media: they can offer an order-of-magnitude increase in thermal storage capacity and their discharge is almost isothermal. This allows to store large amounts of energy without significantly changing the temperature of the sheathing. As heat storage takes place in the building part where the loads occur, rather than externally (e.g., ice or chilled water storage), additional transport energy is not needed.

To numerically evaluate the latent storage performance of treated wallboard, RADCOOL, a thermal building simulation model based on the finite difference approach, will be used. RADCOOL has been developed in the SPARK environment in order to be compatible with the new family of simulation tools being developed at Lawrence Berkeley Laboratory. As logical statements are difficult to use in SPARK, a continuous function for the specific heat and the enthalpy had to be found. This report covers the development of a simplified description of latent storage characteristics for wallboard treated with phase change material.

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NOMENCLATURE

α	thermal diffusivity [m^2/s]
β	inclination [-]
c_p	specific heat [kJ/kg K]
Δ	difference [-]
h	specific enthalpy [kJ/kg]
k	thermal conductivity [W/m K]
ρ	density [kg/m^3]
τ	width of the melting zone [K]
T	temperature [°C]
T_m	melting temperature [°C]
y	dependent variable [-]
y'	first derivative of y [-]

Indices

1	solid phase
2	liquid phase

BACKGROUND

Cooling of residential California buildings contributes significantly to electrical consumption and peak demand. The peak cooling load requires utilities to provide peak-power plants and size their distribution network accordingly. For the building owner, the peak-cooling load determines the size of the equipment and the choice of the cooling source. Several steps can be taken to down-size the cooling systems and to be able to switch to low-energy cooling sources:

- incorporate facades which provide an effective shelter from ambient conditions
- install high-efficient thermal distribution systems (e.g., hydronic systems)
- apply thermal conditioning by radiation rather than by convection
- provide thermal mass, and
- utilize low-energy heating and cooling sources.

Large thermal storage devices have been used in the past to overcome the short-comings of alternative cooling sources or to avoid high demand charges. Buildings designed to make use of thermal storage include features which increase thermal mass. These may be used for storage only or may serve both as storage and as structural elements. Several structural materials satisfy the requirements for sensible heat storage; including concrete, steel, adobe, stone and bricks.

Latent heat storage uses a phase change material as a storage medium. This concept is particularly interesting for lightweight building construction. During transition in phase — freezing, melting, condensing, and boiling — the material absorbs or releases large amounts of heat with little or no change in temperature (E-Source, 1993). Applications typically involve liquid/solid transitions. The PCM is solidified when cooling resources are available and melted when cooling is needed (see **Figure 1**). PCMs have two important advantages as storage media: they can offer an order-of-magnitude increase in heat capacity and their discharge is often almost isothermal (Feustel et.al., 1992).

With the advent of phase change material (PCM) implemented in gypsum board, plaster or other wall-covering material, the thermal storage can be part of the building's structure. This allows the storage of high amounts of energy without changing the temperature of the sheathing. Since storage takes place in the building part where the loads occur, rather than externally, additional transport energy is not needed. With more than 7 billion square meters of plaster board produced annually in the U.S., PCM-treated wallboard could have a significant impact on the utility peak. At the same time, it would help to moderate temperature swings and enhance comfort in homes (E-Source, 1993).

Phase change material can only store energy, but not remove it. In passive applications of structural thermal storage, the heat is being released into the room as soon as the room air temperature falls below the phase change temperature. This heat release mechanism keeps the surface temperatures of the room envelope at the melting temperature level for a long time. This has

certain advantages for the heat transfer mechanism during the discharge of the thermal storage and further complements the use of night-time air to flush the building.

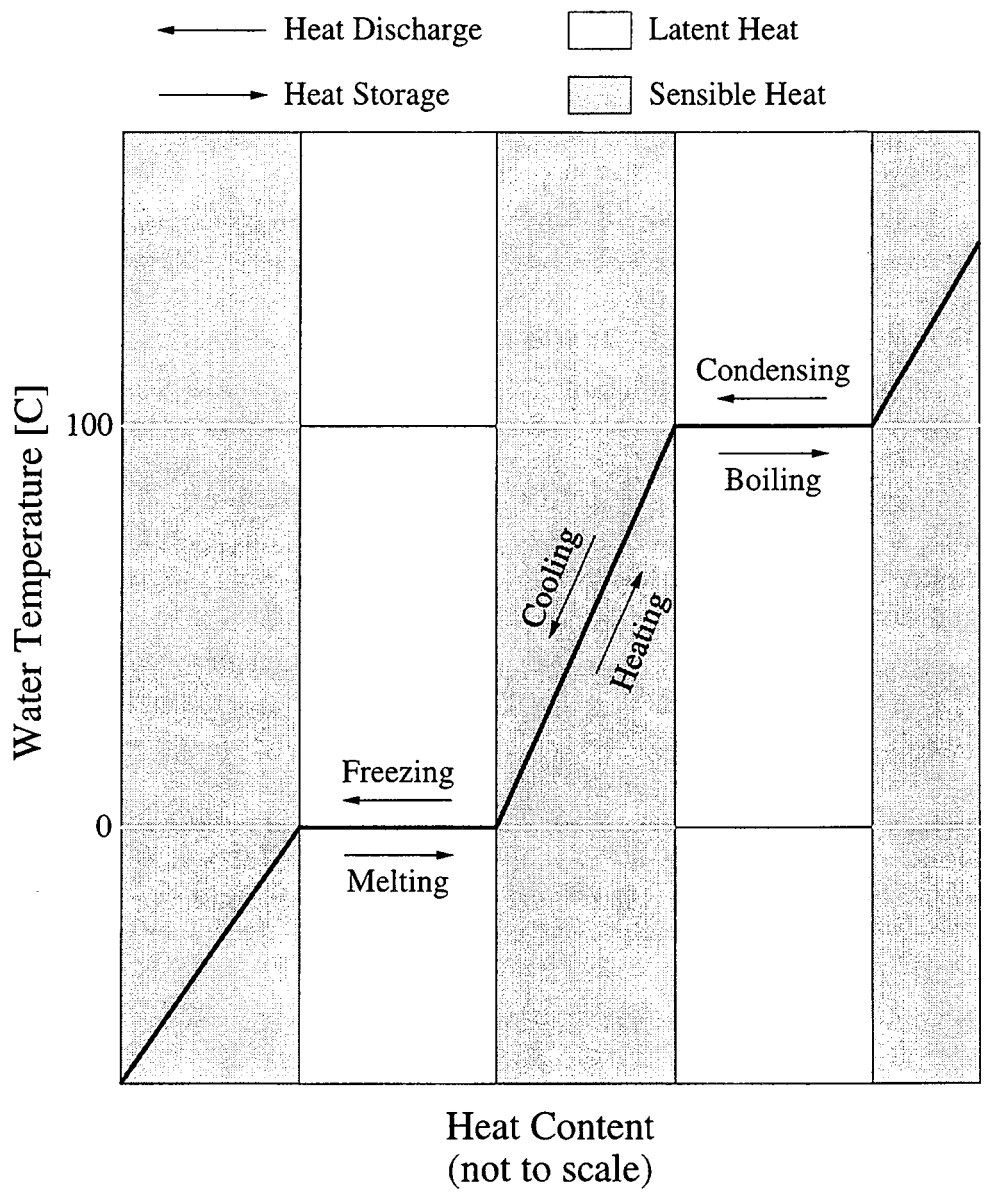

Figure 1: *Phase Change Material Water (E-Source, 1993)*

Besides the passive application, treated wallboard can be coupled with a hydronic loop. Combining continuous discharge and phase change material allows the discharge of thermal energy storage without "dumping" the energy back into the conditioned space.

Previous Research

Research on phase change technology integrated into the building structure as thermal storage for heating and cooling of residential buildings started at the Dayton Research Institute in 1982 (Salyer and Sircar, 1990). The program objectives were to define a cost-effective, environmentally safe, solid-to-liquid PCM which melts and freezes sharply and concurrently at about 25°C and to develop methods by which the PCM could be incorporated into building materials.

Both research goals have been achieved. A suitable low-cost linear alkyl hydrocarbon PCM has been defined, and methods of containing the PCM to eliminate leakage and problems of expansion in melting and freezing have been developed. Processes whereby this PCM could be incorporated into plaster board either by post-manufacturing imbibing of liquid PCM into the pore space of the plasterboard or by additive that could be incorporated into the wet stage of plasterboard manufacture have been developed and tested in detail. (Salyer and Sircar, 1993).

In order to reduce cost, a blend of n-paraffin carbon chains of different lengths below and above 18 carbon atoms (K-18), which melts and freezes almost exactly at 25°C, replaces the more expensive C-18. The PCM is mechanically being mixed into precipitated process silica to make dry powders that remain soft and conformable above and below the melting temperature of the PCM.

Containment costs and attendant problems have been a major problem with many PCM systems developed in the past. In the imbibing process, PCM is imbibed directly into finished plasterboard by immersion in a bath of liquid PCM. Up to 30% of composite weight of PCM can be imbibed in less than 10 minutes. Long-term tests performed by Oak Ridge National Laboratory suggest that little change regarding the PCM properties would be anticipated for wallboard exposed to prolonged use in a normal housing environment (Salyer and Sircar, 1993). Adhesion of paint and joint compound remains unaffected by the presence of the paraffin (Tomlin and Heberle, 1990).

As all organic PCM will continue to burn in a normal air atmosphere after ignition, there could be a severe fire hazard related to PCM-treated wallboard. Two methods tested have shown promising results in eliminating the fire hazard for treated wallboard: limiting the amount of PCM to 15% to 20%, and sequentially treat the plasterboard with PCM and with an insoluble fire retardant.

STORAGE POTENTIAL

Residential Buildings Applications

A piece of sheetrock (0.0125x1.22x2.44m) containing 15% phase change material, has the approximate storage capacity of 277 Wh (93 Wh/m^2). For a detached house with 170m^2 floor area the area covered by wallboard accounts for approximately 370m^2. This translates into a storage capacity of more than 34

kWh, or 9 ton-hours storage capacity. With this amount of passive storage in a house, for most California climates it should be possible to avoid compressor cooling.

Commercial Buildings Applications

If all internal walls and the ceiling of a two-person office (16 m^2) are covered with sheetrock containing PCM (approx. 52 m^2), the thermal storage amounts to 5 kWh (or 1.4 ton hours). The treated sheetrock could store 78 Wh/m^2 floor area for a four hour period, which in non-residential buildings with a reasonable facade and shading devices, should be sufficient to store most of the cooling peak-load imposed by the ambient conditions.

Outlook

While these back-of-the-envelope calculations show very promising results, they do not provide us with the information about the dynamic response. As the phase change material is embedded in the sheetrock, heat to be stored has to reach the "pockets of thermal storage". Although we know that the driving force for heat transfer is the temperature difference, we do not know how much the temperature in the room will increase before a sudden cooling load increase will be absorbed by the walls. The dynamics of the storage process and the response of the heated room determine whether PCM is sufficiently removing the energy from the occupied space.

The correct sizing of the HVAC system and the capacity of the thermal storage are essential in order to minimize part-load operation of the chiller (HVAC oversizing) or overheating the space (HVAC under-sizing).

As mentioned above, the peak-load determines the necessary provision of generated power capacity, the size of the electrical grid necessary, and the size of the HVAC system (and therefore its price, part-load performance and the demand charges). Reduced duct sizes also reduce space requirements for vertical shafts and for plena.

THERMAL PERFORMANCE

Physical Properties of Treated Wallboard

Table 1 shows the physical properties for wallboard as measured by Oak Ridge National Laboratory (Tomlin and Heberle, 1990).

Only ultra-pure paraffins melt and freeze sharply at a given temperature. Mixtures of PCM show a region of temperatures where melting takes place. Results from experimental studies and simulation exercises showed clearly that the treated wallboard does not act like an ideal storage material, which would melt and freeze at a specific temperature. Comparison between measured data and simulation results for the dynamic behavior of a stack of wall boards showed that the best results were obtained if the specific heat as a function of temperature is modeled by the typical triangular shaped curve.

Table 1: *PCM Wallboard Characteristics*

Wallboard	Density kg/m^3	Specific Heat kJ/kg K	Conductivity W/m K	Latent Heat kJ/kg
Conventional	696	1.089	0.173	0
30% PCM	998	1.467	0.232	58.3
20% PCM	800	1.341	0.204	38.9
16% PCM	760	1.299	0.192	31.0
10% PCM	720	1.215	0.187	19.3

Numerical Description of Phase Change

The one-dimensional heat transfer can be described using the heat diffusion equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

A unique mathematical formulation of the melting and solidification is called the Stefan problem. An analytical solution of the problem in the case of an isothermal semi-infinite domain and a discontinuous temperature change at its boundary was found by Neumann (Egolf and Manz, 1994). While crystalline substances and eutectics show a discontinuous transition, many materials (e.g., mixtures) show continuous enthalpy curves as a function of temperature. This leads to a "mushy region" between the solid and the liquid phase.

As the specific heat is taken as the temperature derivative of the specific enthalpy *h*, the specific heat as a function of temperature shows a discontinuity at the melting temperature T_m.

The thermal diffusivity is:

$$\alpha = \frac{k}{\rho c_p}$$

with the specific heat capacity:

$$c_p = \frac{dh}{dT}$$

and the enthalpy:

$$h = \int_0^T c_p(T)dT$$

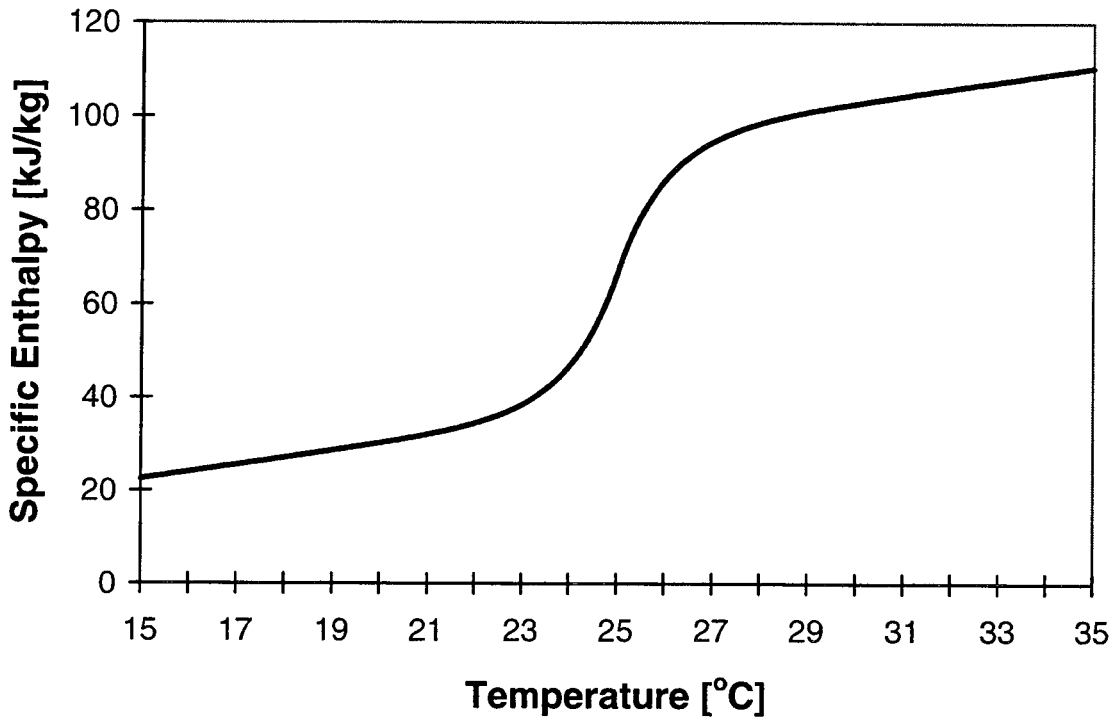

Figure 3: *Specific Enthalpy for Wallboard with 30% PCM;* $\Delta h = 58$ *kJ/kg,* $T_m = 25\,°C$, $\tau_{1,2} = 2$ *K, and* $c_{p_{1,2}} = 1.5$ *kJ/kg K.*

The task is to find a function, which describes the enthalpy development with temperature for a temperature range of 30 K (from 10°C through 40°C) by showing the characteristics described by Egolf and Manz. In order to simplify the task, the enthalpy equation was divided into a sensible part with

$$h(T) = c_{p_{1,2}} T$$

with

$$c_p \neq f(T)$$

and a latent part with

$$h(T) = c_p(T)T$$

For materials which show a symmetrical distribution of the specific heat for the melting region

$$\frac{\tau}{2} = \tau_1 = \tau_2 = \tau_{1,2}$$

the hyperbolic tangent shows some similarity with the mushy region of the

enthalpy curve shown above. With

$$y = \tanh(x) = \frac{\sinh(x)}{\cosh(x)} = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

for the latent heat and

$$y' = [\tanh(x)]' = \frac{\cosh^2(x) - \sinh^2(x)}{\cosh^2(x)} = 1 - \tanh^2(x) = \frac{1}{\cosh^2(x)}$$

for the derivative, representing the specific heat. **Figure 4** shows the hyperbolic tangent and its first derivative for the range of x from -6 to +6.

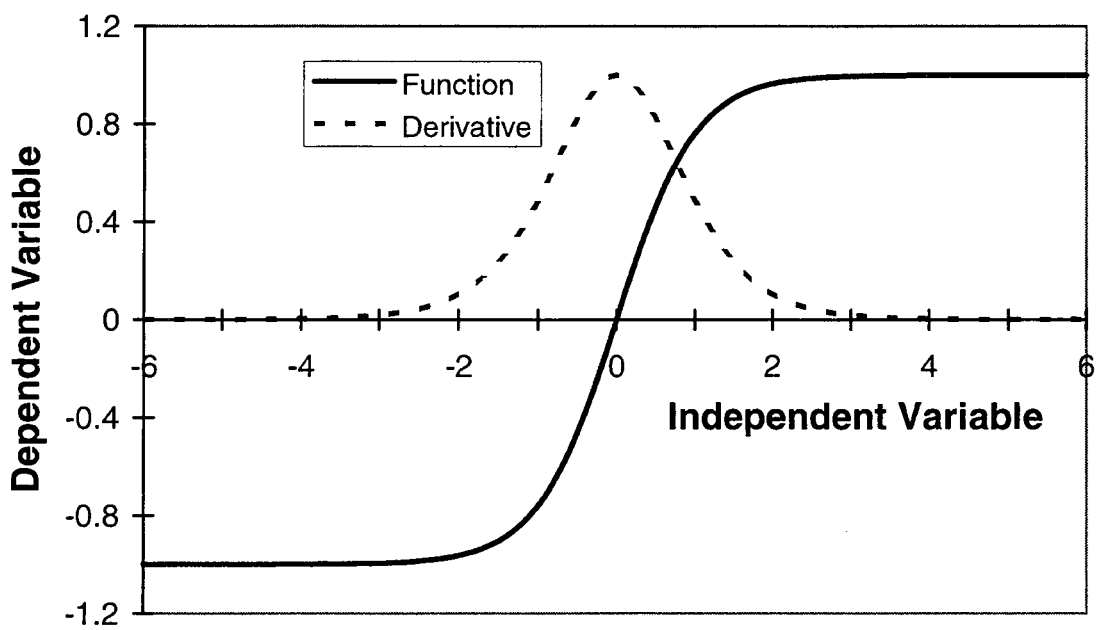

Figure 4: *Hyperbolic Tangent and its First Derivative*

The value of the function changes in a relatively small range of the parameter and the first derivative shows the typical triangular form of the specific heat in the melting region.

With these simplifications, the enthalpy can be described as

$$h(T) = c_{p,const}T + \frac{h_2 - h_1}{2} \times \left\{1 + \tanh\left[\frac{2\beta}{\tau}(T - T_m)\right]\right\}$$

and as the specific heat capacity is the first derivative of the specific enthalpy, we obtain:

$$c_p(T) = c_{p,const} + \frac{h_2 - h_1}{2} \times \frac{\frac{2\beta}{\tau}}{\cosh^2\left[\frac{2\beta}{\tau}(T - T_m)\right]}.$$

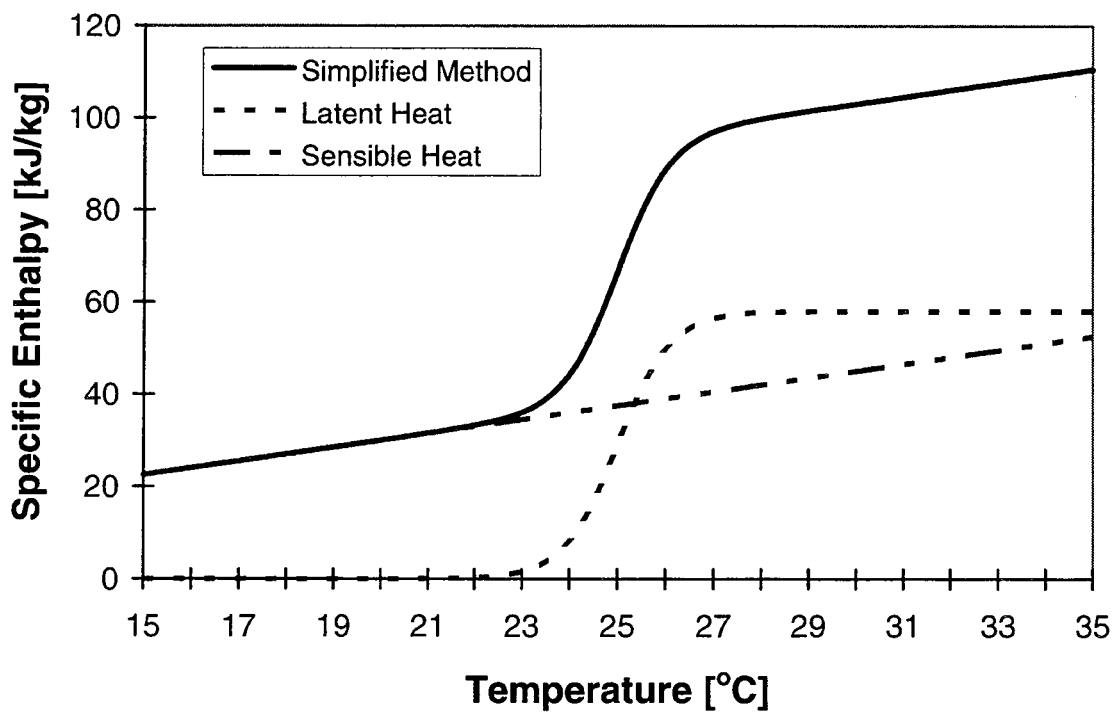

Figure 5: *Specific Enthalpy described by Hyperbolic Tangent for* $\Delta h = 58$ *kJ/kg,* $T_m = 25\,°C$, $\tau = 2$ *K, and* $c_p = 1.5$ *kJ/kg K.*

Figure 5 shows the specific enthalpy as a result of adding the linear sensible enthalpy $h(T) = c_{p,const}T$ to the latent enthalpy represented by the hyperbolic tangent. The inclination $\beta = 1.4$ has been determined by comparison with results from the equation provided by Egolf and Manz.

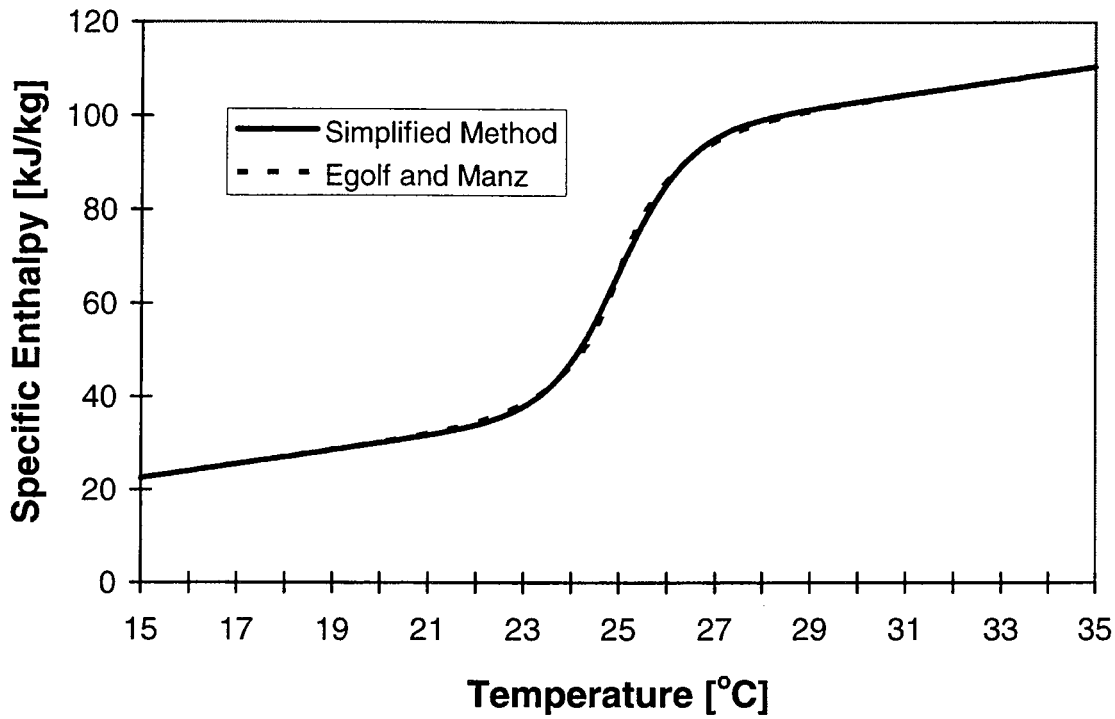

Figure 6*: Comparison between the Specific Enthalpy calculated by Egolf and Manz and by the Simplified Method*

Figure 7 shows the performance of the simplified function for different width of the melting range. With $\tau_{1,2} = 0.1K$, the curve becomes very steep and hardly shows the characteristic rounding above and below the melting temperature. For $\tau_{1,2} = 1K$, the function is slightly steeper in the melting range than the curves described in Figures 2 through 5. A melting range of 20K ($\tau_{1,2} = 10K$) shows a very smooth transition from the solid to the liquid phase of the PCM.

With these options to manipulate the enthalpy change in the melting regime, we are able to describe very pure phase change materials as well as blends of different substances.

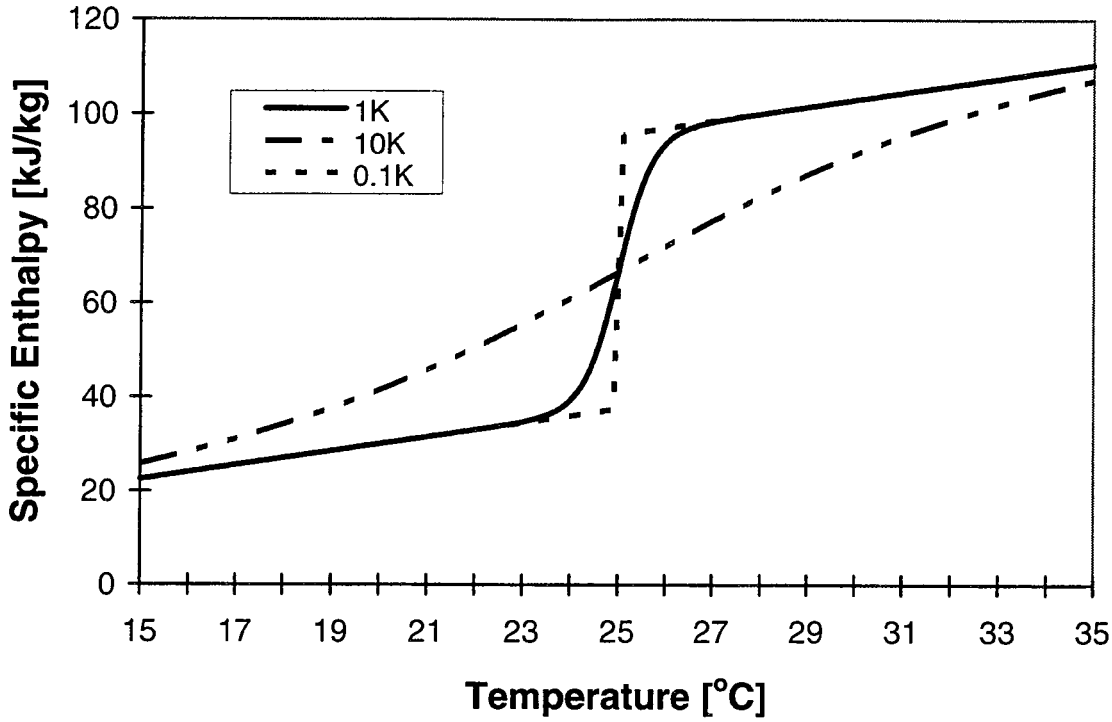

Figure 7: *Specific Enthalpy for different width of the melting zone*

CONCLUSIONS AND FUTURE DIRECTIONS

Based on the numerical description for the latent storage of phase change material with a symmetrical mushy region, a hyperbolic function was used to describe the enthalpy as a function of temperature. With the first derivative of the enthalpy describing the specific heat, a steady function is available to express the varying specific heat in the temperature range relevant for building physics.

This finding allows incorporating the latent storage term into the building component modules developed for the thermal building simulation program RADCOOL without significantly changing the structure of the modules. In order to avoid instability of the dynamic performance simulation, short time steps (in the order of minutes) might have to be introduced for the temperature range of the latent storage.

The functional description of the specific heat will be implemented into some of the wall modules available for RADCOOL. Advanced modules tests will be performed to determine the critical time step as a function of the temperature change and the latent storage characteristics. The final goal of the project is to use the model to numerically evaluate the performance of treated wallboard as a measure to down-size HVAC systems in commercial buildings and avoid compressor cooling for buildings located in transition climates.

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