

TWO SOLUTION METHODS OF HEAT TRANSFER WITH PHASE CHANGE WITHIN WHOLE BUILDING DYNAMIC SIMULATION

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ABSTRACT

The aim of the presented work is to compare two solution methods of specific and latent heat transfer in building components e.g. walls, ceilings or floors. The effect of latent heat storage results from one or more layer made from composites with heighten heat accumulation. This additional heat accumulation follows that the selected layer is modified by incorporating Phase Change Materials (PCM) into its porous structure.

The thermal behavior of phase change storage composites has been studied using numerical techniques. Low-temperature thermal wall has been examined as an internal layer of the identical test cells with the same heating and cooling control system, with set points over and under phase change temperature range. This strategy caused the storing and releasing of heating energy from phase change material (PCM) composites. The temperature of composites and latent heat flux have been estimated using the refined ESP-r system with two additional PCMs modeling procedures. First procedure is based on the so-called "Effective Heat Capacity" method, introduced additional, temperature dependent functions of material capacity. The second method the so-called "Additional Heat Source" method assumed some internal heat source will correspond to latent heat stored or released by material.

Both methods have been implemented in an ESP-r system and applied for building components. The behaviour of PCMs is modelled using ESP-r's *special materials* facility. Numerical analyses have been conducted for two types of PCM-composite layers built in multilayer constructions. The temperature results of the one-dimensional heat transfer process for both cases have been compared and discussed.

INTRODUCTION

The numerical solution methods of heat transfer with phase change have been discussed by Fox (1975), Fuzeland (1980), Crank (1981), Voller & Cross (1983) and Pham (1985). The preferred two methods of finite difference solution are enthalpy or temperature. First of them is characterized by highly

non-linear temperature – enthalpy dependence and explicit scheme is usually unstable. The second is represented by small and width peak of capacity (temperature function). The calculation in some cases, may "jump", the phase change temperature range. This paper proposes both methods, the first so-called "effective heat capacity" which does not suffer from the drawback mentioned above and the second "Additional Heat Source" which requires a relatively short time step to avoid this change phase "missing" and allows a stable numerical solution.

Beginning in the early 1990s, the Department of Building Physics and Building Materials, Technical University of Lodz began investigating organic phase change materials that could be incorporated into traditional building materials: gypsum or ceramic. A lot of experimental analyses and investigation was done using Differential Scanning Microcalorimeter (Romanowska & Jablonski 1995, Klemm 1995) and the results showed considerable thermal energy storage potential. In 2001 the first steps in integration of PCM modeling with whole building dynamic simulation were done in cooperation with Energy System Research Unit, University of Strathclyde, Heim & Clarke (2003). For the purpose of numerical analysis the so-called "Effective Heat Capacity" and "Additional Heat Source" methods, have been taken on and compared. Several subsequent numerical studies estimated energy savings potential and in reduced surface and resultant temperature as well as temperature fluctuations inside building components. Heim & Klemm (2003) and Heim & Clarke (2004) reported the possibilities of PCM for the reduction of heating energy in buildings. Heim (2004) estimated the reduction of temperature fluctuation in transparently insulated storage walls.

PCM COMPOSITES

Thermal energy is generally stored as specific or latent heat. In the former case, the temperature of the medium changes during charging or discharging of the storage, whereas in the latter case the temperature of the medium remains more or less constant since it undergoes a phase transformation. Benard et al. (1985) have presented an experimental comparison of latent and specific heat within thermal walls.

Traditional storage systems, such as a rock-bed, a massive wall etc., not only uses an exclusively specific heat capacity but also give rise to several problems including high cost, excessive mass and undesirable temperature fluctuations. If, however, traditional building constructions are combined with Phase Change Material (PCM), additional latent heat of the phase change is used to increase thermal capacity of the material. Additionally, the phase change is usually almost isothermal, thus providing an excellent means of temperature control.

The utilization of PCMs in active and passive solar buildings has been the subject of interest since their first reported application in the 1940s (Lane 1983). Any PCM composite will comprise two components: a chemical, organic or inorganic compound that undergoes a phase transition within a desired operating temperature range, and a porous structure that acts as a containment for the heat storage substance. In a building context, pure organic or inorganic PCMs can be impregnated into the porous structure of traditional construction materials such as gypsum, concrete or ceramic, which are normally used as an internal surface lining. The thermal performance of different organic (e.g. paraffins, fatty acids etc) and inorganic (e.g. salt hydrates) chemical compounds have been analyzed (Abhat 1983, Hawes et al. 1993, Romanowska & Jablonski 1995, Klemm 1995), with the results demonstrating that organic materials are more thermally stable and easier to encapsulate.

The storage effect of different PCM configurations may then be analysed for the specific context parameters. Few building simulation programs had the refined PCM models at the commencement of the present work, the main objective of which was to modify the existing ESP-r program (Clarke 2001) to include phase-change phenomena. This would make it possible to model and simulate advanced active or passive building elements incorporating PCMs arbitrarily located within a multi-layered construction.

For the purpose of this work 1,5cm inner surface layer made from hypothetical PCM composite was considered. The phase change temperature range for that composite material was 1 Kelvin with melting temperature 20°C and latent heat of phase change at 65000 kJ/kg.

COMPARISON OF TWO METHODS

In first, so-called, “Effective Heat Capacity Method” heat capacity is treated as a function of temperature in phase change temperature range (between melting and solidification). Calculation process is controlled for phase change materials by both: temperature and total latent energy. Below melting temperature the material is fully discharged and additional energy is stored as specific heat. During the phase change

temperature range, temperature fluctuations of the material are limited by almost isothermal, melting or solidification process. Temperature equal to or over solidification temperature is possible only for fully loaded state. Therefore, the material can be out of phase change temperature range only in two cases: when it is fully charged or discharged (figure 1).

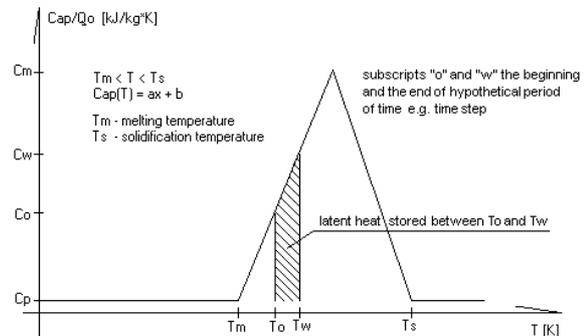


Figure 1. Graphical representation of “Effective Heat Capacity Method”.

The second method the so-called “Additional Heat Source” it assumed some internal heat flux corresponding to latent heat stored or released by material. This flux is temperature dependent in phase change temperature range and it is negative when it stores the heat or positive when the material releases energy. The latent heat flux equals 0 when the material is out of phase change temperature range – below melting or over solidification temperatures (figure 2).

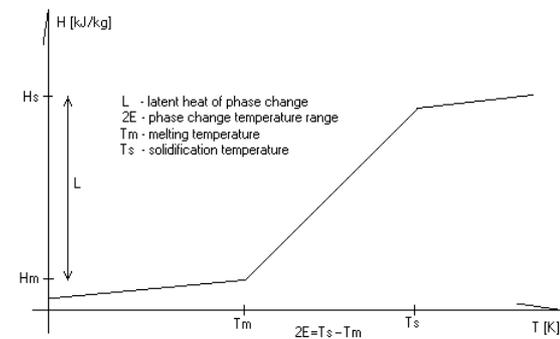


Figure 2. Graphical representation of “Additional Heat Source Method”.

MODELLING PCM COMPONENTS

In the 1980s the first simulation code for a passive solar structure incorporating phase change materials was proposed by a group from Oak Ridge National Laboratory (Drake et al. 1987). This tool allowed a definition of a single room with the wallboard modified by PCM. However, this model suffered from drawbacks, like some simplistic assumptions: constant infiltration, unstratified room air, no additional internal heat sources were considered. The mathematical model based on enthalpy method was validated by comparison with data from an experimental passive solar structure. The heat transfer through the wall was treated only as one-

dimensional. The further research on the application the enthalpy method to solve the heat transfer problems with change of phase has been continued by Peippo et al. (1991). A great deal of research work has been done by a group from Concordia University, Canada (Hawes et al. 1993, Athienitis et al. 1997), who compares numerical results with the measurements from outdoor tests. Jokisalo et al. (2000) build a 3D wall component model able to carry out thermal simulations of building structures containing PCM combined with a single room model within TRNSYS. Finally, Heim and Clarke (2004) refined the ESP-r system by incorporating phase change materials (PCM) modeling based on an effective heat capacity method.

The heat transfer processes in the PCM structures are complex, especially when the chemical compound is in the transition stage. During the phase change process (melting or solidification), the PCM encapsulated in a porous building material can exist in three states: solid, liquid and ‘mushy’ (two-phase). Additionally, the thermal properties of a matrix of construction material are different from the constituent properties. To simplify the mathematical model, the following assumptions were made:

1. The PCM-gypsum composites are treated as a body of uniform equivalent physical and thermal properties, principally specific and latent heat, density and thermal conductivity.
2. The heat transfer process across the PCM-gypsum board is considered as one-dimensional.

The ESP-r control volume approach was adapted to describe the physical elements of the PCM model using ESP-r’s zones and networks elements, (Clarke 2001) and the effective heat capacity method to describe phase change phenomena (Heim 2002). Some initial applications of the method within ESP-r and initial results for gypsum composite are presented elsewhere: (Heim 2002, Heim & Clarke 2003). The exact, detailed description of the model is presented in Heim 2003.

Effective Heat Capacity

The so-called “Effective Heat Capacity Method” represents additional capacity of the material by the function of temperature during change of phases. This function has a narrow and finite width peak between melting and solidification temperatures. The exact dependence is easy to obtain from laboratory measurements and can be approximated by a simple function of additional heat capacity.

The differential equation of transient heat conduction with variable thermo-physical properties is given by:

$$\frac{\partial}{\partial t} \rho(T) \mathbf{h}(T) = \nabla \cdot [\lambda(T) \nabla T(\bar{r}, t)] + g_s(\bar{r}, t) \quad (1)$$

where T is temperature, ρ density, h enthalpy, λ conductivity and g_s sensible heat generation rate.

When

$$\frac{\partial \rho}{\partial t} \approx 0 \quad \text{and} \quad \frac{\partial \mathbf{h}}{\partial t} = \frac{\partial \mathbf{h}}{\partial T} \frac{\partial T}{\partial t} = C_{eff}(T) \frac{\partial T}{\partial t}$$

equation (1) becomes:

$$\begin{aligned} \rho(T) C_{eff}(T) \frac{\partial T(\bar{r}, t)}{\partial t} &= \\ &= \nabla \cdot [\lambda(T) \nabla T(\bar{r}, t)] + g_s(\bar{r}, t) \end{aligned} \quad (2)$$

where C_{eff} is the effective heat capacity.

For the non-linear problem (in the phase change temperature range) defined by equation (2), the Goodman transformation (Samarskii and Vabishchevich 1995) can be used to remove the temperature dependent, effective heat capacity, C_{eff} , outside the differential operator by defining a new dependent variable:

$$v = \int_{C_s}^{C_l} C_{eff}(T) dT$$

where C_s is the heat capacity in solid phase, and C_l the heat capacity in liquid phase.

Heim & Clarke (2004) presented some applications of the effective heat capacity method within ESP-r.

Additional Heat Source

The so-called “Additional Heat Source Method” assumed that some internal heat sources correspond to latent heat stored or released by material. This source represents the enthalpy changes of PCM layer when phase change process appears.

The differential equation of transient heat conduction with additional latent heat source is given by:

$$\begin{aligned} \frac{\partial}{\partial t} \rho(T) \mathbf{h}(T) &= \\ &= \nabla \cdot [\lambda(T) \nabla T(\bar{r}, t)] + g_s(\bar{r}, t) + g_L(\bar{r}, t) \end{aligned} \quad (3)$$

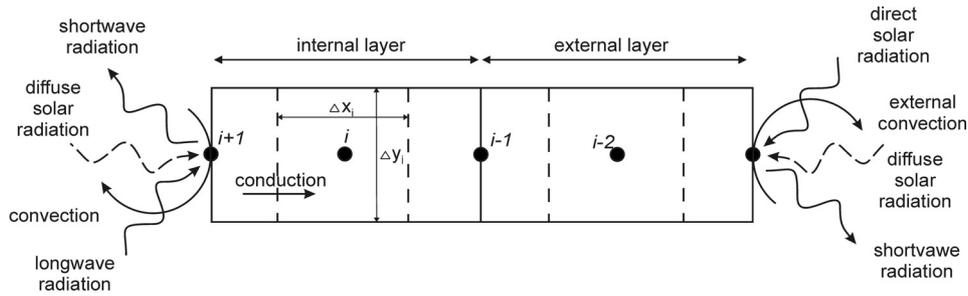
where T is temperature, ρ density, h enthalpy, λ conductivity and g_s specific heat generation rate and g_L temperature dependent, additional latent heat generation rate.

When

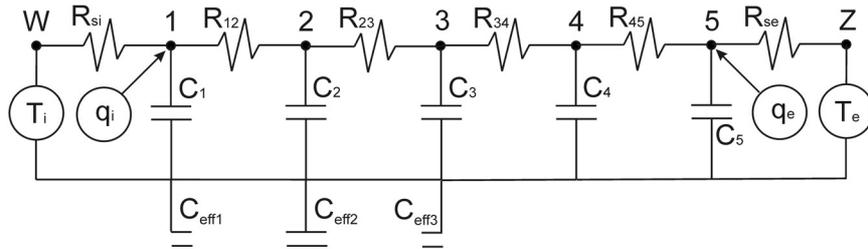
$$\frac{\partial \rho}{\partial t} \approx 0 \quad \text{and} \quad \frac{\partial \mathbf{h}}{\partial t} = 0 \quad \text{and} \quad g_L(\bar{r}, t) = f(T)$$

equation (1) becomes:

$$\begin{aligned} \rho(T) \mathbf{h}(T) \frac{\partial T(\bar{r}, t)}{\partial t} &= \\ &= \nabla \cdot [\lambda(T) \nabla T(\bar{r}, t)] + g_s(\bar{r}, t) + f(T) \end{aligned} \quad (4)$$



Effective Heat Capacity



Additional Heat Source

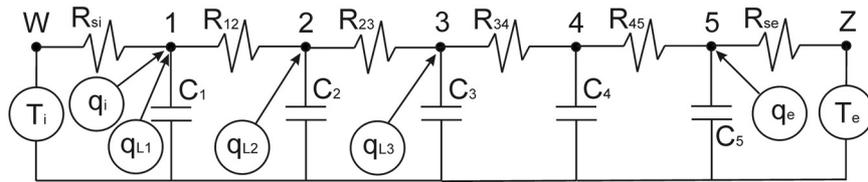


Figure 3. The Control Volume discretization of hypothetical two layers partition.

where $f(T)$ is given by:

$$f(T) = -\rho \frac{\partial H}{\partial T}$$

and H represents additional latent heat of phase change, stored or released by component.

IMPLEMENTATION

Within ESP-r, PCMs were modeled using the concept of special materials (Kelly 1998). Special materials were introduced to ESP-r as a means of modeling active building elements that have the ability to change their thermo-physical properties in response to some external influence (e.g. electrochromic glazing and photovoltaic components). The special material functions of ESP-r may be applied to a particular node within a multi-layer construction. Any node defined as a special material is then subjected to a time variation in its basic thermo-physical properties.

Both methods have been implemented in ESP-r system and applied for building components. The ESP-r multi-layered constructions represent the solid elements which make up the building fabric and provide the physical boundaries to the thermal zones. Considering the application of the control volume

principle to the fundamental heat transfer process, conduction, convection and radiation occurred in every solid element. Each surface layer of the construction can be represented using three control volumes: a homogeneous material volume, a surface volume and a mixed property volume, located at the boundary with the next layer of material. The schematic of two-layers partition with the internal layer made from PCM-composites is shown in fig. 3.

PROBLEM DEFINITION

The main objectives of the presented study are:

1. to apply both methods within a whole building dynamic simulation to model thermal zones bounded by internal layer of the construction,
2. to compare this two methods and study the internal surface temperature history inside the thermal zone.

The thermal properties of the material considered in this study are listed below. The hypothetical material with melting temperature 20°C and latent heat of phase change 65000kJ/kg has been considered. Figure 4 represents the schematic view of a single test cell covered from inside by a thin 1,5cm PCM's component. Two identical zones, one with PCM

composites and one with ordinary material (specific heat only) were tested. During the test, the room air temperature was ideally controlled and set to a high set point of 30°C during the first half a day (0:00 a.m. to 12:00 noon) and to a low set point of 10°C for the rest of the time (12:00 to 0:00 at midnight). On the other side of the layer the adiabatic boundary conditions have been assumed.

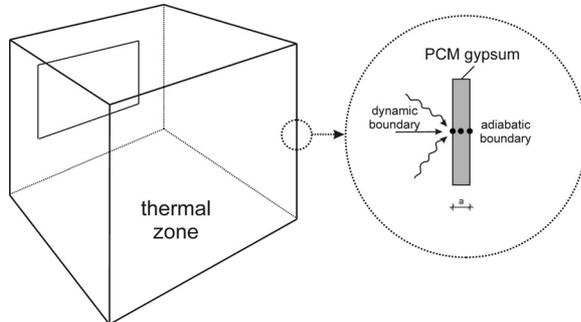


Figure 4. View of the analysed building model with external partition made from PCM-composite.

NUMERICAL ANALYSIS

The history of the PCM composite's surface temperature have been calculated using different models. The analysis has been done using long (60 minutes) and short (1 minute) time steps. Results were compared with traditional material with specific heat that corresponds with specific heat of gypsum board. Figure 5 represents surface temperatures for all cases, where:

EHCM – Effective Heat Capacity Method

AHSM – Additional Heat Source Method

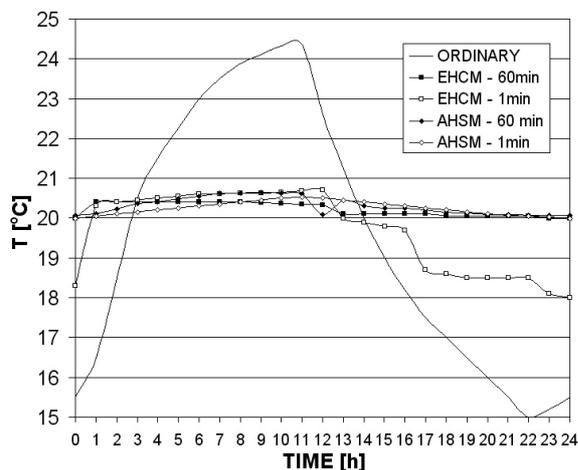


Figure 5. Surface temperature history.

The internal surface is highly exposed to a daily, periodical temperature fluctuation. The phase change process inside the wallboard allows a portion of energy to be stored as latent heat. The surface temperature differs about 4K from ordinary material. Daily temperature fluctuation under dynamic conditions is less than 0,5K for both methods. A

more pronounced temperature fluctuation is seen for the Effective Heat Capacity Method for very short time step, about 1 minute.

SUMMARY

This study is a contribution to the integration of latent heat storage materials within whole building dynamic simulation using two different approaches. The Effective Heat Capacity method and Additional Heat Source method has been successfully applied within whole building dynamic simulations. The results of the numerical analysis have confirmed some slight differences between both methods. The numerical models, implemented in ESP-r to calculate the effect of phase change required further refinements and experimental validation.

All results presented in this paper concerns hypothetical PCM-composite with theoretical thermophysical properties assumed by the author to compare two solution methods.

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NOMENCLATURE

- T – temperature [°C]
 ρ – density [kg/m³]
h – enthalpy [J/kg]
 λ – conductivity [W/m K]
 g_s – specific heat generation rate
 g_L – latent heat generation rate
 C_{eff} – effective heat capacity [J/kg °C]
 C_s – heat capacity in solid phase [J/kg °C]
 C_l – heat capacity in liquid phase [J/kg °C]
 T_m – melting temperature [°C]
 T_s – solidification temperature [°C]