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MODELLING OF LATENT HEAT STORAGE IN PCM MODIFIED COMPONENTS

MODELOWANIE AKUMULACJI CIEPŁA UTAJONEGO W KOMPONENTACH MODYFIKOWANYCH MFZ

Abstract

Due to latent heat storage potential, phase change materials can be implemented in building materials to improve energy performance and thermal comfort. Nevertheless, the phase change effect is quite a complex phenomenon for numerical modelling and different methods can be used to estimate the results of latent heat storage. This paper presents a brief overview of the existing numerical methods and a short description of two most frequently used ones. Authors also investigated the capabilities of phase change modelling by three simulation tools. This work is a part of a wider research project which aims to find optimal solution of façade construction with the implementation of PCM. The choice of a proper numerical method was considered the first step to achieve this goal.

Keywords: phase change material, latent heat, thermal simulation

Streszczenie

W artykule przedstawiono skrócony przegląd metod modelowania numerycznego zjawisk przemiany fazowej oraz możliwości oceny akumulacji ciepła utajonego w komponentach modyfikowanych materiałami fazowo zmiennymi (MFZ). Scharakteryzowano również metody obliczeniowe trzech programów symulacyjnych umożliwiających modelowanie MFZ. W wyniku analizy oceniono zasadność wykorzystania poszczególnych metod do realizacji szerszego projektu mającego na celu znalezienie optymalnego rozwiązania fasady.

Słowa kluczowe: materiały fazowo zmienne, ciepło utajone, symulacje energetyczne

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Nomenclature

C – heat capacity [J/kgK]
H – enthalpy [J/kg]
k – thermal conductivity [W/mK]
L – latent heat [J/kg]
ρ – density [kg/m^3]
t – time [s]
T – temperature [K]
Subscripts:
eff – effective
M – melting
S – solidification

1. Introduction

Nowadays, incorporation of phase change materials (PCMs) within construction components and building elements is increasingly being considered and tested. Heat storage systems and heat capacity of construction materials are the main factors that determine energy efficiency of building envelopes which are highly exposed on solar radiation. Thermal capacity of such components can be increased with phase change materials impregnated in wallboard, microencapsulated or placed in the interspace between two glass sheets. Latent heat energy storage depends mainly on the amount of PCM, its position, melting point and heat of fusion.

During the last decade, the number of simulations and tests were carried out to investigate the performance of PCMs incorporated into building materials. The evaluation of phase change materials performance is a very complex phenomenon and necessitates the implementation of numerical methods to calculate non-linear thermal properties of PCM. Nevertheless, since it was stated that convective heat transfer in PCMs can be neglected [1], governing equations can be reduced to the energy conservation equation:

$$\frac{\partial(\rho H)}{\partial t} = \nabla(k \nabla T) \tag{1}$$

The classification of numerical algorithms for phase-change phenomena description proposed by Idelsohn [2] presupposes a division into two groups: front tracking methods (fixed mesh, variable mesh, moving mesh, moving boundary element) and fixed domain methods (apparent heat capacity, enthalpy based formulation, fictitious heat flow, freezing index, discontinuous integration). The former group of methods is usually used to solve Stefan problem, while methods from the second group give the possibility to model mushy zone (region with solid and liquid phase).

On the other hand, Verma [3] classified numerical models of latent heat thermal energy storage as based on first or second law of thermodynamics. First law models do not include the temperature at which the heat is supplied and the time of the heat storage and release. Nevertheless, second law models should complement – not replace – first law models [4].

Despite the selection of a specific numerical algorithm, the choice of a numerical method for approximating the solution is also crucial for the accuracy of the results. The most commonly used method is the finite-difference method which allows to approximate derivatives by Taylor Series expansion. It can be achieved by explicit, implicit or Crank-Nicholson method, using forward, backward or central difference at time, respectively. Due to non-linear dependence of heat capacity on temperature, which is used to estimate the latent heat storage during phase change, the application of the explicit scheme can cause errors. One of the recommendations leading to increased accuracy of the results is to reduce the calculation time step [5]. Moreover, rapid changes in thermal properties of PCMs can be calculated more precisely by the implicit method. It involves in solution both the current and the previous state of the system in each calculation step.

The most commonly known and used methods are effective heat capacity, enthalpy method and the combination of both.

2. Numerical methods

2.1. Effective heat capacity method

Latent heat storage during phase change can be evaluated using effective heat capacity method. In that method, enthalpy is represented by effective heat capacity – temperature dependence:

$$H = \int_{T_M}^{T_S} C_{eff}\, dT \tag{2}$$

It can be assumed that density change is negligible with time, thus the equation (1) can be expanded as:

$$\frac{\partial(\rho H)}{\partial t} = \rho \frac{\partial(H)}{\partial T}\frac{\partial(T)}{\partial t} = \rho C_{eff} \frac{\partial T}{\partial t} \tag{3}$$

which implies, the governing equation for PCM can be expressed as:

$$\rho C_{eff}(T)\frac{\partial T}{\partial t} = \nabla(k\nabla T) \tag{4}$$

where:

$$C_{eff}(T) = \begin{cases} C_p & T_S < T < T_M \\ \dfrac{L}{T_S - T_M} + C_p(T_M) & T_M \le T \le T_S \end{cases} \tag{5}$$

As stated before, calculation can be proceeded using explicit or implicit method of solution. Due to sharply changing function of effective heat capacity, proper assumption of the time step size is crucial while using explicit method. Calculation step has to be small to avoid the situation when the temperature “jumps” past the solidification point in one step and latent heat is ignored [6]. Nevertheless, effective heat capacity method allows us to use implicit discretization scheme which, in that case, is unconditionally stable [7]. Through the use of DSC method for measuring effective heat capacity, in the equation (4) the only unknown variable is the temperature.

2.2. Enthalpy method

The second method for latent heat storage evaluation is enthalpy method, which estimates heat capacity in form of its integral form $H(T)$ with respect to temperature**.** This method assumes that enthalpy is a sum of sensible and latent heat [8]:

$$H(T) = h(T) + Lf(T) \tag{6}$$

where:

$$h(T) = \int_{T_M}^{T_S} C_p dT \tag{7}$$

and liquid fraction is given as:

$$f(T) = \begin{cases} 0 & T < T_M \\ \dfrac{T - T_M}{T_S - T_M} & T_M \le T \le T_S \\ 1 & T > T_S \end{cases} \tag{8}$$

One of the main advantages of that method is the applicability of the above equations directly to the three phases. There is no need to track over moving phase front and mushy zone can be easily modelled. The temperature is evaluated in each time step and values of thermo-physical properties can be determined precisely.

a) b)

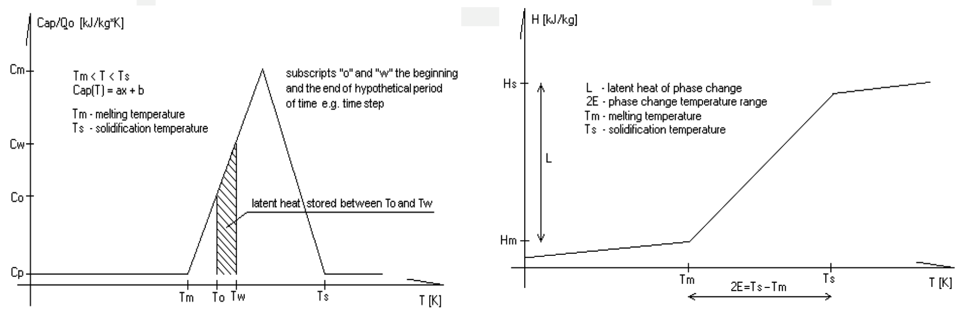

Fig. 1. Graphical representation of a) effective heat capacity method, b) enthalpy method [14]

3. Simulation tools

3.1. EnergyPlus

Latent heat storage in EnergyPlus can be evaluated by modified version of the enthalpy method. The implemented algorithm allows us to calculate heat capacity on the basis of enthalpy-temperature function in each time step [9]:

$$C_{eff} = \frac{H_{i,new} - H_{i,old}}{T_{i,new} - T_{i,old}} \tag{9}$$

Solution of one-dimensional conduction finite difference (CondFD) algorithm can be proceeded using Crank-Nicholson or fully implicit scheme [10]. Despite the fact that the model includes both phase-change enthalpy and temperature dependent thermal conductivity, it is not possible to take into account the effect of hysteresis on the heat capacity [11].

3.2. TRNSYS

TRNSYS is a modular simulation software consisting of many subroutines, which allows to implement different calculation methods. It is possible to implement new module TRNSYS Type [12, 13] or use the active layer tool in TRNSYS Type 56. As investigated by Klimes [8], both enthalpy and effective heat capacity methods are applicable in TRNSYS software. Nevertheless, it is necessary to implement numerical model of PCM in MATLAB (in case of the former method) or in the form of a stand-alone module in the C++ programming language.

3.3. ESP-r

Energy performance of PCM modified components can be evaluated using an active materials subroutine implemented in ESP-r software [14]. Through the definition of the special material properties latent heat storage is estimated on the basis of the effective heat capacity method. Despite the highly non-linear dependence of heat capacity and temperature, this function can be substituted by a linear one:

$$C_{eff}(T) = aT + b \quad T_M < T < T_S \tag{10}$$

where:

$$b = \frac{L}{\Delta T}$$

4. Discussion and further work

In this paper, three simulation tools calculating non-linear thermal properties of PCMs have been described and discussed. Authors also presented and compared two numerical methods of assessing the effect of phase change and latent heat generation: effective heat capacity method and enthalpy method. The former method allows us to determine the temperature change on the basis of heat capacity measured through differential scanning calorimetry, while the second one describes enthalpy by integrating the heat capacity with respect to temperature. The main assumptions and limitations of both methods were pointed.

This study is a part of a wider research project devoted to optimization of the energy-efficient construction of the façade. Effectiveness of PCM is quite sensitive to external weather conditions and indoor temperature. Hence, the assessment of specific solution should be made taking into account all variables and using appropriate simulation tools. Furthermore, the accuracy of obtained results should match the scope of the analysis – analysis of a particular element, entire façade or whole building analysis. Authors investigated the possibilities of application mentioned numerical methods and concluded that further experimental investigations are necessary to confirm the accuracy and applicability of presented methods.

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References

[1] Zalba B., Marin J.M., Cabeza L.F., Mehling H., *Review on thermal energy storage with phase change: materials, heat transfer analysis and application*, Applied Thermal Engineering, 23, 2003, 251-283.

[2] Idelson S.R., Stori M.A., Crivelli L.A., *Numerical methods in phase-change problems*, Archives of Computational Methods in Engineering, 1994, 49-74.

[3] Verma P., Varun, Singal S.K., *Review of mathematical modelling on latent heat thermal energy storage systems using phase-change material*, Renewable & Sustainable Energy Reviews, 12, 2008, 999-1031.

[4] Dutil Y., Rousse D.R., Salah N.B., Lassue S., Zalewski L., *A review on phase-change materials: Mathematical modeling and simulations*, Renewable & Sustainable Energy Reviews, 2011, 15 112-130.

[5] Almeida F., Zhang D., Fung A.S., Leong W.H., *Comparison of corrective phase change material algorithm with ESP-r simulation*, 12th Conference of IBPSA, Sydney 2011.

[6] Pham Q.T., *A fast, unconditionally stable finite-difference scheme for heat conduction with phase change*, Heat Mass Transfer, 28, 1985, 2079-2084.

[7] Klimes L., Charvat P., Ostry M., *Challenges in the computer modeling of phase change materials,* Materials and technology, 46, 2012, 335-338.

[8] Sharma A., Tyagi V.V., Chen C.R., Buddhi D., *Review on thermal energy storage with phase change materials and applications*, Renewable & Sustainable Energy Reviews, 13, 2009, 318-345.

[9] Pedersen C.O., *Advanced zone simulation in EnergyPlus: Incorporating of variable properties and phase change material (PCM) capability*, Proceedings: Building Simulation 2007.

[10] Tabares-Velasco P.C., Christensen C., Bianchi M., *Verification and validation of EnergyPlus phase change material model for opaque wall assemblies*, Building and Environment 54, 2012, 186-196.

[11] Evola G., Marletta L., Sicurella F., *A methodology for investigating the effectiveness of PCM wallboards for summer thermal comfort in buildings,* Building and Environment, 59, 2013, 517-527.

[12] Ibanez M., Lazaro A., Zalba B., Cabeza L F., *An approach to the simulation of PCMs in building applications using TRNSYS*, Applied Thermal Engineering, 25, 2005, 1796-1807.

[13] Kuznik F., Virgone J., Johannes K., *Development and validation of a new TRNSYS type for the simulation of external building walls containing PCM*, Energy and Buildings, 42, 2010, 1004-1009.

[14] Heim D., Clarke J.A., *Numerical modeling and thermal simulation of PCM-gypsum composite with ESP-r*, Energy and Buildings, 36, 2004, 795-805.