Determination of Optimal Heat-Storage Thickness of Layer for "Smart Wall" by Methods of Nonlinear Heat Conduction Equations for Phase-transition Materials

I Pospelova
Building and Architecture Institute, Irkutsk National Research Technical University, 83, Lermontov str., Irkutsk 664074, Russia

E-mail: pospel@istu.edu

Abstract. The article suggests an original way of keeping heat load and its compensation for a microclimate system by proposing the "Smart Wall". The construction consists of specially combined composite materials including phase-transition materials. The method for determination of the layer thickness is proposed for a certain accumulation time. Varying the thickness and composition of the layer it is possible to achieve a low amount of the thermal conductivity coefficient and to obtain various functional characteristics of fences.

1. Introduction
Smart House is a modern residential building, organized for the most comfortable living in it through the use of high-tech devices. A modern smart house involves a number of systems that are able to recognize specific situations and adequately respond to them, while such systems can monitor the normal functioning of other systems and processes in accordance with a predetermined algorithm, and all of them are integrated in a united complex. But in the presence of a large number of different equipment, there is a problem in simplifying and delegating the management functions to the objects themselves. That object can be a smart coating for walls or any structures which is able to maintain the required of the temperature potential.

Specially modeled composite coating "Smart Wall", including phase change material and vacuum capsule allows compensating smoothly for temperature fluctuations and leveling the load on the system to maintain a comfortable temperature, avoid the occurrence of the dew point.

One way to maintain of the temperature potential is the transition of a substance from one phase to another, occurring by the temperature changes, pressure, or under the influence of some other external factors at the boundary of heat transfer process, or in the thickness of the material. There are phase transitions with a sharp change in the density and entropy of matter, called phase transitions of the first kind. In this case, the first derivatives of thermodynamic potentials change rapidly by the intensive parameters of the system, and the most important, primary extensive parameters changes: specific volume, amount of stored internal energy, concentration of components, etc. For phase transitions of the second kind, the density and entropy of a substance changes continuously at the transition point, and the heat capacity, compressibility and other similar characteristics experience a jump. As a rule, the symmetry of the phase also changes accordingly. Density and internal energy do not change, so
such a phase transition can be invisible to the unaided eye. A jump is experienced derivatives of
temperature and pressure: Heat capacity, coefficient of thermal expansion, various sensitivity, etc.

For heat transfer processes it is important the first kind of phase transition. During a time, a phase
transition does not occur immediately in the entire volume of matter, but gradually with the extraction
(or intake) a certain amount of energy. Unlike crystalline bodies, kinetic and photon theories of heat
are quite applicable to amorphous bodies [1].

The test material is a solidified suspension containing matrices with a phase transition material and
capsules with an insulating substance, and contains up to 90% of the phase-transition material. The
test material is located at the boundary of the heat exchange zone and aligns of the heat gain or
absorbs an excess heat. So as physical and textural properties of synthesized suspensions are under
study, we use the data on the specific reduced factor of thermal diffusivity of such materials [2-4]. To
determine the total amount of such a material, it is sufficient to determine the required amount of
latent heat, and to determine the thickness of the layer and the size of the coating of such material,
mathematical modeling of the process is necessary.

2. Mathematical modeling of the nonlinear model of diffusion heat transfer process
Mathematical models of processes of heat and mass transfer in substance with phase transitions are
nonlinear systems of differential equations. An analytic solution of the one-dimensional nonlinear heat
conduction problem is called the Stefan problem. Even with constant coefficients of the equation due
to the presence in it of Stefan type conditions on the boundary of a phase transition model is nonlinear,
and the main method of solving are numerical methods. Only in discrete particular cases is it possible
to use the analytical method. So, it may obtain so-called self-similar solutions, which are characterized
by the similarity of spatial distributions of the sought-for quantities at different instants of time. Such
decisions are put to one-dimensional problems in the half-space with constant boundary and initial
conditions. Self-similar solutions allows to describe the experimental processes at times and at big
distances from the boundary that the influence of the initial and terminal conditions disappears, but at
times and distances sufficiently small that the system is still far from the limiting state [3,5].

Let the liquid medium is spreading a half-space $x > 0$ and accept at $t < 0$ the temperature of all
layers of the liquid is the same and equal to $u > u^*$, where $u^*$ - liquid solidification temperature.
Commonly it will assume $u^* = 0$.

From the time $t = 0$ at the border $x = 0$ a constant temperature maintains $uc < 0$ below the
crystallization temperature $u^*$. In this case at $t > 0$ near boundary surface a layer of solid phase shows
up, the thickness of which increases over time (Figure 1). Crystallization front $x = \xi(t)$ at any time
separates the solid phase from the liquid phase, moving at a some speed $v = d\xi/dt$ to the direction of
the liquid phase. At the problem statement $\xi(0) = 0$.

![Figure 1. Direction of the crystallization front.](image)
The heat of the phase transfer, which is emitted after crystallization of the liquid, takes away due to the thermal conductivity of the solid phase through the boundary surface $x = 0$.

Clearly identifying the moving crystallization front, we designate by the index "1", it is values related to the solid phase, and index "2" - to the liquid phase. Then, assuming that the properties of the medium change unevenly in the phase transition, write the heat equation for two phases:

$$\frac{\partial u_1}{\partial t} = \alpha_1 \frac{\partial^2 u_1}{\partial x^2} \quad t > 0, \quad 0 < x < \xi(t)$$

$$\frac{\partial u_2}{\partial t} = \alpha_2 \frac{\partial^2 u_2}{\partial x^2} \quad t > 0, \quad \xi(t) < x < \infty$$

(1)

where $\alpha_1$ and $\alpha_2$ - thermal diffusivity of the solid and liquid phases, respectively.

Taking into account that at the initial moment of time the liquid phase exists only, the initial condition for the problem is written in the form:

$$u_2(x,0) = \text{const}, \quad x > 0$$

(2)

The boundary conditions of the problem can be formulated as follows:

a) at the boundaries of the region

$$u_1 = u_2 = \text{const} < 0, \quad x = 0$$

$$u_2 \to u_0 = \text{const} > 0, \quad x \to \infty$$

(3)

b) on the front of phase transition

$$u_1 \big|_{z = \xi - 0} = u_2 \big|_{z = \xi + 0} = 0$$

$$k_1 \frac{\partial u_1}{\partial x} \big|_{x = \xi - 0} = k_2 \frac{\partial u_2}{\partial x} \big|_{x = \xi + 0} = \rho q^* \frac{d\xi}{dt}$$

(4)

where $q^*$ - Latent heat of crystallization, referred to the unit mass of the solid phase.

Using a self-similar variable $\eta = x/(t)^{1/2}$ (Boltzmann transform), we give the equations (1) and to ordinary differential equations for functions $u_1(\eta)$ and $u_2(\eta)$.

Integrating twice and returning to the variables $x$ and $t$, we present the solutions of equations (1) in view:

$$u_1(x,t) = A_1 + B_1 \Phi \left( \frac{x}{2a_1 \sqrt{t}} \right), \quad t > 0, \quad 0 < x < \xi(t)$$

$$u_2(x,t) = A_2 + B_2 \Phi \left( \frac{x}{2a_2 \sqrt{t}} \right), \quad t > 0, \quad 0 < x < \xi(t)$$

(5)

According the boundary conditions (3), we find

$$A_1 = u_-, A_2 + B_2 = u_0$$

(6)

We note that the initial condition (2) will also be satisfied.

From condition (4) on the phase transition front, i.e. at $x = \xi(t)$ following
\[ A_1 + B_1 \Phi \left( \frac{\xi(t)}{2a_1 \sqrt{t}} \right) = 0; \quad A_2 + B_2 \Phi \left( \frac{\xi(t)}{2a_1 \sqrt{t}} \right) = 0. \quad (7) \]

Each of these conditions can be fulfilled for any \( t > 0 \) only if arguments of the function \( \Phi(z) \) in these equations do not depend on time. But this is possible if

\[ \frac{\xi(t)}{t^{1/2}} = \alpha = \text{const} \quad (8) \]

Thus, accurate within a certain constant \( \alpha \), representing the coefficient of thermal diffusivity, the law of motion of the phase transition front

\[ \xi(t) = \alpha \sqrt{t} \quad (9) \]

And its speed

\[ v = \frac{d\xi}{dt} = \alpha / 2 \sqrt{t} \quad (10) \]

It decreases with time, as the layer of the solid phase increases and thickens.

Thus, a nonlinear heat conduction problem with a phase transition can be used for modeling the accumulation and consumption of heat in a non-stationary heat exchange process [6-9], including in the wall and structures of the smart house, as well as technological processes of melting, directed crystallization, growing of single crystals and the production of specified structures of semiconductor materials. Using mathematical models, such processes can be optimized for various factors.

3. Simulation by finite element method

Several variants of the structure for composite materials for determining the boundary and the speed of the phase transition have been simulated. Based on the velocity development of the transition boundary, it became possible to model the thickness of an Smart Layer that has inclusions with a phase transition material. The thickness of the melting zone \( x \) depends on the time \( t \) and the thermal diffusivity coefficient \( \alpha \).

Depending on the time of heat development, we can determine the necessary layer thickness. Combined composite materials with a melting point of 30-50 °C were used for the research. Let's take the time to get heat from solar energy and heat recuperation from the room, during which energy accumulates during the day, and at night a discharge equal to the minimum value of 4 hours. Table 1 shows the calculation of the required thickness of the Smart Layer depending on the composition of the combined materials of the layer. In this case, the goal was to achieve a total wall thermal conductivity coefficient up to 0.3 W/m²°C.

| Model Number | Specific thermal diffusivity of the coating layer, \( a \times 10^{-6} \), m²/c | Coating Thickness, mm | Remark |
|--------------|--------------------------------------------------------------------------------|----------------------|--------|
| 1            | 0.08                                                                         | 9                    | Capsules with the addition of a paraffin-like substance |
| 2            | 0.22                                                                         | 26                   | With the addition of air capsules |
| 3            | 1.19                                                                         | 142                  | With the addition of heat transfer metal |
| 4            | 0.082                                                                        | 9.8                  | With the addition of synthetic polymers |
The author developed the design of the heat accumulator (Pospelova I.Yu., Pospelova M.Ya. Patent for Utility Model "Heat Accumulator-exchanger" № 145327, Registered on August, 2014), with application of the calculated layer no more than 1 cm. The accumulator can be used in systems with solar energy, in recuperation plants. The average specific heat of fusion of the composite layer is 120 kJ/kg. Proceeding from this, the minimum economy of day energy will be 50W*hours.

4. Conclusions
The layer of heat-accumulating composite material applied to the walls makes it possible to average heat gains and heat losses by enclosing structures and to make "Smart Walls" that will reduce excess heat dissipation and compensate an additional heat loss without the cost of electricity systems and without any energy at all. In addition, it will be possible to avoid the "dew point" in structures. It will increase the hygienic and exploitative properties of buildings and structures.

References
[1] Fedotov P and Kochetkov A 2016 Thermal photonics About phase transitions of the first and second kind J. Science vol 85 68TVN516
[2] Glagolev K and Morozov A 2007 Physical thermodynamics (Moscow: Moscow State Technical University of Bauman) p 272
[3] Martinson L and Malov Yu 2002 Differential equations of mathematical physics (Moscow: Moscow State Technical University of Bauman) p 368
[4] Kosova E and Lebedev V 2006 A model of a structural first-order phase transition close to the second J. of Fundamental Research 2 pp 70–1
[5] Gorelik S and Dashevsky M 2003 Material science of semiconductors and dielectrics (Moscow: MISIS) p 480
[6] Landau L and Lifshitz E 1976 Statistical physics (Moscow: Nauka) p 584
[7] Patashinskii A and Pokrovskii V 1982 Fluctuation theory of phase transitions (Moscow) p 381
[8] Elesin V and Kashurnikov V 1997 Physics of phase transitions (Moscow: MEPI Publishing House) p 180
[9] Yakovlev V, Yakovlev M and Shterenberg A 2008 Phenomenological description of phase transitions and critical phenomena (Samara: State Techn Univ, Samara) p 166