Numerical simulation of processes in the latent-heat thermal energy storage tank

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Abstract. This paper has proposed a computer model for numerical calculations of heat flows in regular rhombic packed bed of capsules with phase change material. The mathematical model of heat transfer in a capsule is based on finding a zero-dimensional solution to the Stefan problem, considering the influence of convective flows arising in the liquid phase. To take into account the heat transfer due to the convective component in the liquid phase in the capsule, the effective thermal conductivity coefficient is calculated. An experimental dependence has been applied to describe the heat exchange conditions of the coolant and the capsule wall. The calculation is reduced to finding the temperature of the coolant after passing one layer of packed bed. The resulting temperature is the input parameter for calculating the next layer. This operation is repeated until the calculation is made for all layers of packed bed. The numerical calculation has been performed in the mathematical software Scilab. According to the proposed model, the results of calculating the temperature of the coolant after passing the storage device correlate well with the experimental data for a thermal energy storage device with spherical capsules filled with paraffin.

1. Introduction
In 2018, cooling premises accounted for only 4.6% of total building maintenance costs according to company estimates DNV GL. According to their forecasts, by 2050, energy share for cooling premises will increase to 12% roughly divided equally between residential and commercial buildings. All this will be observed with an increase in energy consumption for maintenance of premises by 25% by 2050 [1].

Separately, it is worth highlighting the countries of Africa with their high daytime temperatures and rapid population growth. According to forecasts, by 2040, there will be more than 1 billion people living in sub-Saharan Africa who need cooling. This means that cooling should become one of the factors determining the extent of future energy demand.

By 2030, Africa is planning to achieve universal electrification. As the incomes of African households grow, they will increasingly purchase household appliances such as refrigerators, washing machines and telephones. Wealthier households will purchase indoor cooling systems. Thus, in the region, the number of air conditioners is expected to increase almost six times to about 45 million by 2040, and their operation will increase electricity consumption by 40 TWh [2]. All of the above forecasts assume an increase in demand for cooling systems and a significant increase in the total energy consumption for their operation.

In residential premises, there is observed cyclical consumption of cold. The peak consumption occurs during the daytime, while the systems are idle at night. In situations of this kind, one of the best
optimization methods is the introduction of latent-heat thermal energy storage (LHTES) into cooling systems [3,4]. Their use reduces the peak equipment loads since part of the load will be removed by the stored energy (Fig. 1). This allows the use of installations of lower power. Charging LHTES at night at double rates reduces energy costs.

At the same time, a number of renewable energy sources are cyclical. For example, charging and discharging LHTES can be carried out using the energy of the sun and night radiation cooling [5-9]. However, for the efficient operation of air conditioning and refrigeration systems using LHTES, it is necessary to select the optimal design parameters. The power of the installation, the duration of the charge/discharge cycle, the operating temperatures and the type of active substance depend on these parameters. One of the ways to calculate them is to perform computer simulation of heat and hydraulic flows in LHTES.

![Graph of consumed thermal energy.](image)

**2. Review of Literature**

With the development of energy-saving technologies and the renewable energy industry, the study of LHTES has become more active [10]. Many studies [11-14] investigates the processes occurring in thermal energy storage with phase change material (PCM) and their designs.

A review article [11] discusses work on melting/solidifying PCM in a single spherical capsule. It analyses constrained melting (solid PCM fixed inside the vessel), unconstrained (unfixed) melting and solidification. Methods for intensifying heat transfer inside the capsule by using orthogonal ribs are presented.

Review paper [12] considers the work on intensification of heat transfer in LHTES. Both experimental tests and results of numerical simulation are described.

In paper [13], various numerical models used to predict the characteristics of storage in the packed bed are considered. Some useful correlations which allow us to quantify the main physical phenomena associated with packed bed operation and simulation are presented and compared. The investigated correlations make it possible to calculate the heat transfer coefficients of liquid/solid and liquid/wall, the effective thermal conductivity and the pressure drop in packed bed.

Paper [14] presents various features of the design, operation and performance of LHTES with packed bed. Various numerical models that are used to predict the characteristics of thermal energy storage in the packed bed are presented.

Simulation is often carried out in CFD packages. They are based on the methods of finite volumes and elements. With the help of them, one can get accurate and visual results. However, the calculation with their use requires significant computational and time costs due to the large nonlinearity of the properties of PCM. The most popular way to calculate such systems is the enthalpy-porosity method.

Paper [15] describes modelling in thermal energy storage unit with phase change material in ANSYS FLUENT where the enthalpy-porosity method is used. For calculations with its help, it was required to
purchase a commercial version of Ansys Fluent, to build a computational grid with a size of 9.3x10⁹. The calculation was carried out on a workstation with 32 Intel Xeon-core CPUs and 32 GB RAM.

Paper [16] proposes an efficient thermal conductivity model for modelling the entire LHTES reservoir. However, it describes processes only for cubic packed bed. The creation of such a structure requires additional effort.

3. Mathematical model

In this paper, a mathematical model is proposed for describing heat flows in the packed bed of capsules of PCM. To describe the processes occurring inside the capsules, a mathematical model for numerical calculations of solid-liquid phase transitions based on the zero-dimensional solution of the Stefan problem was used. In this method, the unknown quantities are the average radius of the position of the phase transition boundary \( r_m \) and the temperature of the capsule shell \( T_c \). It is assumed that the phase transition occurs at a constant temperature \( T_m \).

The equation describing the phase boundary:

\[
\frac{dr_m}{dt} = \frac{T_c(t) - T_m}{R(t)} \frac{1}{\rho_f A_m(t) [L + c_f(T_c(t) - T_m)]}
\]  

(1)

where \( c_f \) and \( \rho_f \) – specific heat and density of the liquid phase respectively, \( A_m \) – phase boundary area being calculated through the average radius \( r_m(t) \), \( R \) – thermal resistance of the liquid phase interlayer calculated in accordance with [17].

\[
R(t) = \frac{r_c - r_m(t)}{4\pi r_m(t) k_{ef}}
\]  

(2)

where \( r_c \) – inner radius of the shell.

The effective coefficient of thermal conductivity \( k_{ef} \) is calculated by the formula:

\[
k_{ef} = \begin{cases} 
  k_f, & Pr < 1000 \\
  0.18 \cdot k_f \cdot (Gr \cdot Pr)^{0.25} & \text{otherwise}
\end{cases}
\]  

(3)

where \( k_f \) – thermal conductivity of the liquid phase, \( Gr \) – Grashof number, \( Pr \) – Prandtl number.

\[
Gr = \beta_f \cdot g (r_c - r_m(t))^3 \frac{T_c - T_m}{\nu^2}
\]  

(4)

where \( \nu \) – kinematic viscosity of the liquid phase, \( g \) – gravitational acceleration.

For \( T_i(t) \), the equation is written under the assumption of a uniform temperature field of the shell:

\[
C \frac{dT_i(t)}{dt} + \frac{T_i(t) - T_m}{R(t)} + \alpha S(T_i(t) - T_{i+1}) = 0
\]  

(5)

where \( C \) – total heat capacity of the shell, \( \alpha \) – heat transfer coefficient, \( S \) – area of the outer surface of the capsule, \( T_{i+1} \) – temperature of the coolant before passing through the capsule layer.

Then it is necessary to draw up a system of differential equations. To represent this equation (5) as follows:

\[
\frac{dT_i(t)}{dt} = -\frac{1}{C} \left( \frac{T_i(t) - T_m}{R(t)} + \alpha S(T_i(t) - T_{i+1}) \right).
\]  

(6)

From formulas 1 and 6, a system of ordinary differential equations is formed. To find its solution, the 4th order adaptive Runge-Kutta method is used [18].

In a regular rhombic packed bed, to describe the conditions of heat exchange between the coolant and the walls of capsules with PCM, the experimental dependence proposed in [19] was applied:

\[
Nu = 0.825 Re^{0.62}.
\]  

(7)

For other structures of the packed bed, the dependencies described in [20] can be used.
Reynolds number is calculated by the formula:

$$Re = \frac{D_{cap} \nu \rho}{\eta}$$  \hspace{1cm} (8)

where $D_{cap}$ – diameter of the capsule with PCM, $\nu$ – coolant flow rate, $\rho_{cool}$ – coolant density, $\eta_{cool}$ – dynamic viscosity of the coolant.

The heat transfer coefficient is calculated by the formula:

$$\alpha = \frac{Nu \cdot \lambda_{cool}}{l}$$  \hspace{1cm} (9)

where $\lambda_{cool}$ – thermal conductivity of the coolant; $l$ – outer diameter of the capsule.

Having calculated the average radius $r_m(t)$ and the temperature of the capsule shell $T_c(t)$ with the help of equations (1-6), we find the heat flow from one capsule:

$$q(t) = \frac{T_c(t) - T_m}{R(t)}$$ \hspace{1cm} (10)

Then we calculate the heat flow from one layer:

$$q_i(t) = q(t) \cdot k$$ \hspace{1cm} (11)

where $k$ – number of capsules in one packed bed layer.

The temperature after passing through the $i$-th layer is calculated by the formula:

$$T_i(t) = T_{i-1}(t) - \frac{q_i(t)}{Q_m \cdot C_{pcool}}$$ \hspace{1cm} (12)

where $T_{i-1}(t)$ – temperature of the coolant before passing through the $i$-th layer, $Q_m$ – mass flow rate of the coolant, $C_{pcool}$ – specific heat of the coolant.

The temperature obtained by formula (12) is the input parameter for calculating the next packed bed layer. This operation is repeated for each packed bed layer. The use of this method assumes a uniform temperature field for each individual packed bed layer.

4. Experimental data

To test the mathematical model, paper [21] was chosen as a source of experimental data. In this work, air is supplied to the LHTES tank through the mixing chamber at an initial temperature of 10 °C. Within an hour, the air temperature changes to a constant 35 °C. The diameter of the tank is 34 cm (Fig. 2). The tank contains a regular rhombic packed bed of capsules with PCM (paraffin RT20). Its properties are shown in Table 1. The outer diameter of the capsules is 50 mm, the wall is made of polyethylene with a thickness of 1 mm. The volumetric air consumption is 215 m$^3$/h. The air temperature is recorded at the outlet from the tank.

![Figure 2. Experimental stand [21].](image)
| Thermophysical properties               | Value   |
|-----------------------------------------|---------|
| Melting point (°C)                      | 21      |
| Thermal conductivity (W/m°C)            | 0.2     |
| Specific heat capacity (kJ/kg/K)        | 1.4     |
| Heat of fusion (kJ/kg)                  | 140     |
| Density (kg/m³)                         | 880     |
| Kinematic viscosity (m²/s) × 10⁻³       | 6.25    |
| Coefficient of thermal expansion (K⁻¹)  | 0.001   |

5. Calculation results
Figure 3 shows a graph comparing the air temperature after passing the LHTES. As you can see, there is a significant deviation by 1/3 of the time interval, but this does not significantly affect the final results of calculating the discharge time of the LHTES. The error in calculating the final discharge time of the LHTES amounted to 1.3%. In the remaining time interval, a close fit between the calculation results using the proposed model and the experimental results is observed. The calculation was carried out on Intel Core i5-8600 and 8 GB RAM in the Scilab environment. The calculation time amounted to 276 seconds.

![Figure 3. Comparison with experimental data [21].](image)

6. Conclusions
The article presents a method (mathematical model) for numerical calculations of solid-liquid phase transitions in a rhombic packed bed of a LHTES. The model has a high accuracy in calculating the LHTES discharge time. The calculation time for the proposed model was 276 seconds. The duration of the calculation and its accuracy make it possible to use this mathematical model for the design calculation of air conditioning and refrigeration systems.

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