Calculation of cold accumulators with phase change materials

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Abstract. The paper presents an improved technique (mathematical model) for numerical calculations of solid-liquid phase transitions based on a zero-dimensional solution of the Stefan problem for cases of placing phase change materials in ball-shaped or cylindrical capsules. According to the proposed model, numerical calculations of the liquid phase volume fraction in Scilab have good compliance with experimental data for n-octadecane, and the calculation time is reduced several hundred-fold in comparison with calculations in Fluent.

1. Introduction
It is advisable to use cold accumulation at variable loads of consumers, at large difference in electricity rates during day and night, if there are technical and economic grounds for using renewable energy resources for cold energy accumulation (for example, sun energy and night radiation cooling) [1-5]. For instance, variable cold-supply capacities can be found in production refrigerators in case of large quantities of food supplies that requires cooling or freezing, in air-conditioning systems, which cold consumption during the daytime is usually higher than at night. Peak shaving by accumulated cold allows using refrigerating systems with lower capacity. The accumulation of cold by compressor refrigerators at night at double rates reduces energy costs.

Cold accumulators may use liquids, frozen water ice, phase change materials (PCM) as accumulating medium. The use of PCM reduces the capacity of accumulators by 5-14 times compared to the use of liquids [3]. The advantages of PCM also include constant phase transition temperature, chemical stability and economic efficiency. The specific heat of phase transition plays a major role in energy storage of such cold accumulators. In case of liquid-solid phase transition the accumulator is charged, and in case of reverse phase transition the solid-liquid is used [6].

The PCM can be placed in a cold storage tank in capsules in the form of balls, as well as circular or rectangular pipes. Thus, a coolant circulates in space between capsules [6]. This type of accumulators is most common. The PTS density in the accumulator in ball-shaped capsules makes about 50%, in rectangular pipes – about 90% of the volume [7]. In other cases, the PCM is placed in the accumulator tank, and the coolant circulates inside the pipes of the heat exchanger located in the tank.

2. Study of cold accumulator operation
In order to design cold accumulators with PCM, among other aspects, it is necessary to reliably calculate the processes of liquid-solid and solid-liquid phase transitions corresponding to charging and discharging of cold energy accumulators.

Many works are devoted to the study of thermal energy accumulators and thus related processes during charging and discharging [8-17]. The main calculation method in case of phase transitions is enthalpy-porous approach during numerical solution of the Navier-Stokes system of equations for PCM, which is considered as an incompressible liquid [14-17]. The phase transition boundary is not
directly modeled, which is ensured by the unity of setting equations for solid and liquid phases. Thus, the volume fraction of a liquid phase \( \beta \) depends on temperature \( T \) as follows [14]

\[
\beta = \begin{cases} 
0, & \text{if } T < T_{sol} \\
1, & \text{if } T > T_{liq} \\
\frac{T - T_{sol}}{T_{liq} - T_{sol}}, & \text{if } T_{sol} < T < T_{liq}
\end{cases}
\]

(1)

where \( T_{sol} \) – solidus temperature, \( T_{liq} \) – liquidus temperature.

Change of flow characteristics during phase transition is taken into account by introducing the porous zone in the transition zone, the porosity of which varies from 0 (solid phase) to 1 (liquid phase). The constants of the porous zone are determined during the numerical experiment [18].

The idea of enthalpy approach is to replace the energy of unknown temperature in the equation by enthalpy \( H \) determined through the temperature of phase transition and the liquid phase fraction [15]

\[
H = H_{ref} + \beta L + \int_{T_{ref}}^{T} \text{cd}T,
\]

(2)

where \( H_{ref} \) – enthalpy at relative temperature \( T_{ref} \), \( L \) – heat of phase transition, \( c \) – PCM specific heat. This approach allows the heat of the phase transition to be considered directly in the energy equation

\[
\frac{\partial(\rho H)}{\partial t} + \nabla(\rho \nu H) = \nabla(k\nabla H),
\]

(3)

where \( \nu \) – liquid velocity, \( t \) – time, \( k \) – PCM heat conductivity, \( \rho \) – PCM density. Thermal conductivity and density are fugacity of temperature.

However, the disadvantage of this approach includes the problems with convergence of a strongly non-linear problem for numerical solution, and the large calculation time even for two-dimensional problems.

An alternative can be the approach based on the Stefan problem, where the location of a mobile phase transition boundary is unknown. The boundary conditions at the boundary of solid and liquid phases are defined here. Namely, the temperature continuity condition and the heat flux condition. Such systems of equations are solved analytically for one-dimensional cases when charging an accumulator, since it is not necessary to consider in detail the convective heat fluxes in the liquid phase. The classical solutions to Stefan problem are given in [19-21]. However, the solution in the case of accumulator discharge causes the need to consider heat fluxes in the liquid phase and the natural convection.

3. Calculation methodology

The authors of this paper propose the procedure for calculating heat fluxes during the discharge of accumulators based on a zero-dimensional solution of the Stefan problem for cases of placing PCM in ball-shaped or cylindrical capsules. The average radius of the phase transition boundary \( r_m \) and the capsule shell temperature \( T_c \) are unknown here, as shown in Figure 1. It is assumed that the phase transition occurs at a constant temperature \( T_m \).

![Figure 1. Thermal model of accumulator with PCM.](image-url)
Equation for phase boundary

$$\frac{dr_m(t)}{dt} = -\frac{T_c(t)-T_m}{R(t)} \frac{1}{\rho_f A_m(t)[k+c_f(T_c(t)-T_m)]},$$  (4)

where $c_f$ and $\rho_f$ – specific heat capacity and density of liquid phase, respectively, $A_m$ – area of phase boundary calculated through the average radius $r_m(t)$, $R$ – thermal resistance of ball or cylindrical layer of the liquid phase calculated in accordance with [22]

$$R(t) = \frac{r_c-r_m(t)}{4\pi r_c r_m(t) \kappa_{ef}},$$  (5)

$$R(t) = \frac{1}{2\kappa_{ef}} \ln \frac{r_c}{r_m(t)},$$  (6)

where $r_c$ – inner radius of the shell. The formula (5) is applicable in the case of a ball shell, (6) – for a cylindrical shell. The effective thermal conductivity coefficient $\kappa_{ef}$ is calculated by the formula

$$\kappa_{ef} = \begin{cases} \kappa_f, & \text{Pr} < 1000 \\ 0.18 \cdot \kappa_f \cdot (Gr \cdot Pr)^{0.25} \end{cases},$$  (7)

$$Gr = \frac{b_m \cdot g(r_c-r_m(t))^3}{\nu^2(T_c-T_m)},$$  (8)

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

For $T_c(t)$, the equation is written on the assumption of a uniform shell temperature field

$$C \frac{dT_c(t)}{dt} + \frac{T_c(t)-T_m}{R(t)} + \sigma(T_c(t) - T_a) = 0,$$  (9)

where $C$ – total heat capacity of the shell, $\sigma$ – heat conductivity from the shell to the heat carrier with temperature $T_a$. At larger $\sigma$, the model turns into a model for the known temperature $T_c = T_a$ [23].

4. Results and discussion

Equations (4) – (9) are solved numerically.

In order to verify the developed method, the design values are compared with the experimental ones, which were calculated in the Fluent package using equations (1) – (3) taken from [14] for n-octadecane. In [14], a numerical solution is based on the first order approximation resulting in a computational error. The second order approximation used by the authors of this paper in the numerical solution better corresponds to experimental data. The numerical calculation according to formulas (4) – (9) is performed in Scilab package. The calculation data are shown in Figure 2.

Figure 2. Comparison of calculation data.
5. Conclusion

Figure 2 shows that in fact the calculations of the liquid phase volume fraction done according to the proposed model in the Scilab package coincide with the numerical calculations in the Fluent package, but the calculation time in the latter case increases several hundred-fold. The obtained results also coincide well with experimental data, the discrepancy can be caused by the introduction of thermoelectric converters into capsules throughout the experiments, which was not taken into account in numerical calculations. This makes it possible to use the developed mathematical model in calculation and design of cold accumulators with PCM.

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