On numerical model of one-dimensional time-dependent gas flows through bed of encapsulated phase change material

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\textbf{Abstract.} Mathematical model and numerical method are proposed for investigating the one-dimensional time-dependent gas flows through a packed bed of encapsulated Phase Change Material (PCM). The model is based on the assumption of interacting interpenetrating continua and includes equations of state, continuity, momentum conservation and energy for PCM and gas. The advantage of the method is that it does not require predicting the location of phase transition zone and can define it automatically as in a usual shock-capturing method. One of the applications of the developed numerical model is the simulation of novel Adiabatic Compressed Air Energy Storage system (A-CAES) with Thermal Energy Storage subsystem (TES) based on using the encapsulated PCM in packed bed. Preliminary test calculations give hope that the method can be effectively applied in the future for modelling the charge and discharge processes in such TES with PCM.

\section{1. Introduction}

Thermal Energy Storage (TES) can be considered as a solution of energy conservation problem which arises when the availability for energy does not coincide with demand. TES are applied in solar energy, central air cooling, air heating, waste heat recovery, etc. Phase Change Materials (PCM) are used in these devices to increase storage density. TES with PCM have been achieving lately a high penetration in the market in the areas of thermal protection and thermal inertia \cite{1}.

One of the effective methods to compose TES with phase change is packed bed of PCM enclosed in spherical particles, which are heated (cooled) by the Heat Transfer Fluid (HTF), flowing through it \cite{2}. Last time this construction is adopted for novel Adiabatic Compressed Air Energy Storage (A-CAES). CAES differs from other storage methods, because it is available for high power ranges and energy capacities \cite{3}; CAES is promising technology for energy storage with high reliability, economic feasibility, and low environmental impact \cite{4}. The advantage of A-CAES is that the processes of gas compression and expansion occur adiabatically, so the heat of the compressed air is not lost and remains in the process for using in power generation. These properties make the A-CAES to be the most perspective technology for energy storage. Experimental analyzes and numerical modeling of CAES with PCM in the packed bed are performed in \cite{5-7}; empirical investigations of the fixed and fluidized bed of the PCM blown by the heated air is presented in \cite{8}. Modeling the processes of heat transfer in packed bed of the encapsulated PCM with air as the HTF and validation with experimental data are considered in \cite{9,10}.
Since the problems with phase transitions have analytical solution in limited class of conditions, the numerical methods are developed for these problems [11]. These methods can be separated in two groups: methods with selection of the phase interface and shock-capturing methods. When flow of HTF in the packed bed of the encapsulated PCM is considered, the zone of the phase change is some area, where the transition takes place in every point simultaneously. So, the explicit phase interface is absent, and assumption of the instant phase transition is not actual. It does not allow to apply the known methods of calculating the phase transitions in similar problems.

When typical particle size in the packed bed thermal energy storage is relative small, TES can be considered as a porous medium. Mathematical model and numerical method were developed in [12] and tested in [12-14] for calculating the time-dependent one-dimensional gas flows through the porous heat-evolutional objects with known pressure at the boundaries and unknown gas flow rate. These model and method were modified and applied for simulating the time-dependent cooling processes of two-dimensional heat-evolutional objects [15] and heterogeneous combustion in porous media with unknown oxidant flow rate [16,17].

In the present work the numerical model based on previous results [12] is proposed for modeling the one-dimensional time-dependent gas flow through the packed bed of the encapsulated PCM; some test calculations are carried out.

2. Mathematical model

Let a motionless porous object consist of small balls made from phase change (solid – liquid) material (PCM) enclosed in envelope. Suppose that the porous object is bounded of impermeable non-heat-conductive side walls and is opened at the top and at the bottom. The PCM has its crystallization (melting) temperature $T_m$. When fraction of the PCM is much larger than fraction of the envelope material the last one can be neglected. Specific heat capacity, heat conductivity, density of the PCM are assumed to be constant during and after phase change. A gas is conveyed with known temperature and pressure into the inlet of the object (at the bottom); the gas flows up, changes its temperature as a result of the heat exchange with the particles, and flows out through the object top to the ambient air with known pressure.

Mathematical model is very similar to the previously developed model described in detail in [12]. It is constructed on model of two interactive interpenetrated continua [18] and includes the equations of continuity, momentum conservation, state and energy for each medium:

$$
\begin{align*}
(1-a)\rho_c \frac{\partial T}{\partial t} &= -\alpha(T - T_g) + (1-a)\lambda \frac{\partial^2 T}{\partial x^2} + (1-a)\rho_s \frac{\partial f}{\partial t}, \\
\rho c_p \left( a \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) &= \alpha(T - T_g) + \frac{\partial P}{\partial t} + u \frac{\partial P}{\partial x} + \frac{\mu}{k} u^2, \\
\frac{1-(1-a)\chi}{a^2} \rho \left( a \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) &= -\frac{\partial P}{\partial x} - \rho g - \frac{\mu}{k} u, \\
a \frac{\partial^2 \rho}{\partial t^2} + \frac{\partial (\rho u)}{\partial x} &= 0, \quad P = \rho R T_g, \quad \mu = \frac{c_s}{c_s} \frac{T_g^{\gamma / 2}}{T_g + T_s},
\end{align*}
$$

where $a$ is the porosity, $c_p$ is the specific heat capacity of gas under constant pressure, $c_s$ and $c_d$ are the constants in Sutherland formula, $f$ is the degree of phase change, $g$ is the acceleration of gravity, $k$ is the coefficient of permeability of the porous medium, $L$ is the latent heat of PCM, $P$ is the gas pressure, $R$ is the gas constant, $T$ is the temperature of the PCM, $T_g$ is the temperature of the gas, $t$ is the time, $u$ is the gas filtration velocity ($u = av$, where $v$ is the gas velocity), $x$ is spatial coordinate, $\alpha$ is the constant determining the intensity of the interphase heat exchange, $\lambda$ is the coefficient of the heat-conductivity of PCM, $\mu$ is the coefficient of dynamic viscosity of the gas, $\rho$ is the density of the gas, $\rho_s$ is the density of the PCM, $\chi$ is the coefficient taking into account the inertial interaction of the phases in their relative motion [18].
It should be noted that the equations of motion and continuity of the PCM degenerate and are not included in the system since the PCM is assumed to be motionless with constant density.

The phase change is taken into account in the energy equation of the PCM by addition of the term with function \( f \), which means the degree of phase change. This function is equal to 0 and 1 before and after the phase change respectively, and is unknown a priori when the phase change takes place. On the contrary, the PCM temperature is equal to \( T_m \) during the phase change and is unknown in other cases. Sign at the last term in the equation of energy for PCM is determined by the direction of the phase changing: the upper sign is selected for solidification; the lower sign is selected for melting.

The temperature and the pressure of the gas are known at the inlet of the object, the gas pressure at the outlet is known. Conditions of heat exchange are known on the both open boundaries (bottom and top) of the object. So, the boundary conditions for system (1) can be written as follows:

\[
\begin{align*}
T_s|_{x=a} &= T_{g0}, \\
\frac{\partial T}{\partial x}|_{x=0} &= \beta (T|_{x=0} - T_{g0}), \\
P|_{x=1} &= P_0, \\
\frac{\partial T}{\partial x}|_{x=1} &= \beta (T|_{x=1} - T|_{x=H}),
\end{align*}
\]

where \( P_0, P_a, T_{g0} \) are known values of the pressure and gas temperature respectively, \( \beta \) is the heat transfer coefficient.

To solve system (1) with boundary conditions (2) it is necessary to specify the values of sought parameters at the initial moment of time.

3. Numerical method

System (1) with boundary conditions (2) is solved by finite-difference method on the uniform grid with mesh size \( h \) and time step \( r=hr^2 \), where \( r=const \). The algorithm is based on the previously proposed and tested in [12-14] numerical procedure for computing one-dimensional time-dependent gas flow through the porous object with internal heat-evolutional sources when the gas pressure at the open boundaries of the object is known. The equations of energy and motion are transformed into explicit finite-difference schemes; the continuity equation is written in implicit form and is solved using the Thomas algorithm [19]. The temperatures and the velocity of the gas are determined from the energy and motion equations respectively; the gas pressure is determined from the continuity equation, then the density is determined from the equation of perfect gas state. The boundary conditions for grid functions are defined from (2) trivially. This finite-difference scheme approximates system (1) with the first-order time accuracy and the second-order accuracy in space; the convergence takes place under a certain limitation on \( r \). The main difference between the present method and the one described in [12] is the first equation in (1) (energy equation for PCM), which includes two unknown functions: \( f \) and \( T \). Denoting the variation of time coordinate by superscript and the variation of space coordinate by subscript, let’s write the finite-difference equation of energy for PCM (other equations are the same as in [12]):

\[
\rho c(T_{m+1}^n - T^n_m) = -\frac{\tau a}{1-a}\left(T^n_m - T^n_{gm}\right) + r\lambda(T^n_{m+1} - 2T^n_m + T^n_{m-1}) \pm L\rho c\left(f_{m+1}^n - f_{m}^n\right)
\]

(3)

Explain the feature of the algorithm on an example of the following problem. Before starting moment, the temperature inside the porous object is equal to ambient temperature, which is lower than \( T_m \); the gas does not flow. At the initial time moment, the gas begins to flow into the object inlet at a fixed pressure and temperature, which is higher than \( T_m \). The gas flows up, heats the PCM to the melting temperature, and the phase transition begins after some time. Further heating of solid particles continues after the ending of phase transition until the stabilization of the PCM and gas temperatures. So, the whole process can be divided into three stages. The first stage is the heating of the PCM from initial temperature to the melting temperature; the second stage is the phase transition; the last stage is the further heating of the PCM until the temperature stabilization. Consider the algorithm for calculating \( T \) and \( f \) in every stage. At the first stage \( f \) is equal to 0 according to the definition. So, the last term in (4) is absent, and (3) is transformed into the following explicit scheme for determining \( T \):
\[ T_{m}^{n+1} = \left( 1 - \frac{\tau \alpha}{(1-a)\rho c} \right) T_{m}^{n} + \frac{\tau \alpha}{(1-a)\rho c} T_{gm}^{n} + \frac{r \lambda}{\rho c} \left( T_{m+1}^{n} - 2T_{m}^{n} + T_{m-1}^{n} \right) \]  

(4)

Computations using (4) continues until the melting temperature of the PCM is reached. Than the second stage (the phase transition) begins. The PCM temperature is equal to \( T_{m} \), and left part of (3) is equal to 0. Since the melting is considered, lower sign at the last term in (3) is selected, and \( f \) is explicitly defined from (3):

\[ f_{m}^{n+1} = f_{m}^{n} + \frac{1}{\rho c L} \left( -\frac{\tau \alpha}{1-a} \left( T_{m}^{n} - T_{gm}^{n} \right) + \frac{r \lambda}{\rho c} \left( T_{m+1}^{n} - 2T_{m}^{n} + T_{m-1}^{n} \right) \right) \]  

(5)

Computations using (5) continues until \( f=1 \); than the phase change is completed, and the third stage (further heating of the PCM until the temperature stabilization) begins. The last term in (3) is equal to 0, and scheme (3) is transformed into (4) again.

When solidification is considered, the algorithm is similar except the selection of the upper sign at the last term in (3).

The advantage of the proposed method is that it does not require predicting the location of phase transition zone and can define it automatically as in a usual shock-capturing method. Due to this, the proposed method can be easily extended to 2D and 3D cases.

4. Calculations

The proposed numerical method was implemented and tested on simulation of the gas flow through the packed bed of the encapsulated PCM. The results were compared with results in [20], where simulation of the HTF flow through the bed of microfine particles of the PCM is considered. Air was used as HTF, and paraffin was used as PCM. Comparison between the results of the present numerical simulation and data in [20] is demonstrated in figure 1, which shows the PCM temperature at the outlet (x=2 m) of the porous object. As can be seen from the Figure 1, times of the beginning and the ending of the phase change coincide; times of the stabilization of the PCM temperature are close.

![Figure 1. PCM temperature at the outlet (x=2 m) of the bed versus time for data in [20] (1) and for the present numerical simulation (2).](image-url)
Figure 2 depicts the PCM temperature within the porous object in fixed time for data in [20] and for the present numerical simulation. As seen from the figure 2, both results are rather close. The difference between the results is due to the fact that the applied mathematical model has a number of differences from the model used in [20]. The system of equations (1) takes into account more factors than the model in [20] like heat conductivity in PCM, power of internal forces in the gas etc.

![Figure 2. PCM temperature in time t=2314 s versus the height of the bed for data in [20] (1) and for the present numerical simulation (2).](image)

In the near future, it is planned to modify the proposed numerical model for possibility to calculate the process when the gas velocity at the object inlet is fixed, and then to compare calculated result with experimental data under conditions of fixed gas velocity at the object inlet.

5. Conclusions
On the basis of the mathematical model and numerical method for simulating the time-dependent processes of gas flows through the heat-evolutional porous media with known pressure at the open boundaries and unknown gas flow rate, the mathematical model and numerical method are proposed for investigating the time-dependent one-dimensional gas flows through the packed bed of the encapsulated phase change material. The developed numerical model can be applied for the simulation of novel adiabatic compressed air energy storage system with thermal energy storage subsystem based on using the encapsulated PCM in packed bed. The advantage of the method is that it does not require predicting the location of phase transition zone and can define it automatically as in a usual shock-capturing method.

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