On two-dimensional gas flows through granular phase change material

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Abstract. A novel numerical model is proposed for modelling two-dimensional planar gas flows in granular phase change material (PCM). The mentioned model consists of system of equations based on the classical methods of mechanics of heterogeneous media which is solved by original finite-difference algorithm. Effect of heat transfer with ambient medium on mushy zone propagation in the bed of granular PCM is investigated by means of numerical experiment. It is shown that phase transition speed can decrease significantly near the side walls of the bed in relation to the central region which provides curvature of the mushy zone boundaries and nonuniform melting of the PCM in the bed. Kind of curvature of these boundaries can change in dependence of heat conductivity coefficient of the PCM.

1. Introduction
Phase change materials (PCM) are materials which melt or crystallize at certain temperature and by this way allow to store thermal energy without large temperature change. They are very common in energy conservation and management problems and renewable energy [1]. Such materials are often applied in thermal energy storages (TES) which are used for accumulation energy from the moving heat transfer fluid (HTF). In this case to obtain the stability of the construction the PCM is put in the hermetic capsules or in the spongy granules made from some inorganic material which does not allow the PCM to flow out of the sponge by means of its adsorption properties. Herewith the gas is often used as HTF in the TES. Such thermal storages are applied in novel adiabatic compressed air energy storage (CAES) [2] and in other applications.

Problem of describing the phase change boundaries also known as Stefan problem arises at modelling heat propagation in media which change the aggregate state at certain temperature. This problem complicates when modelling the granular PCM with heat transfer fluid because convection in the fluid provides formation of the region with intermediate state of the material also called mushy zone instead classical phase change boundary. So, the class of the known numerical methods of determination of the phase change boundaries cannot be applied [3]. When modelling the gas flows through bed of granular or capsular PCM two methods of description of the phase transition are usually applied. The first one is related to sharp changing of the specific heat capacity of the material during the phase change [4-6]. The second one is the approach of the mushy zone model [7, 8]; it implies using the additional function – liquid fraction in the PCM [9, 10].
The gas flows through granular PCM can be considered as filtration flows in porous media with energy release sources. Herewith release and absorption of the energy occurs during crystallization and melting respectively. Mathematical model and original numerical method for investigating the one-dimensional time-dependent gas flow through the bed of granular PCM are proposed and tested in [11-13]. The model was validated by means of comparison of the calculation results with experimental measurements which shown good coincidence of data. Influence of gas compressibility on gas flows through bed of granular PCM was investigated in [14, 15]. It was shown that there are regions of values of problem parameters where the gas compressibility can be neglected, but at the same time there are regions of the values where the gas compressibility must be taken into account since it can change the solution significantly. Moreover, the neglect of the gas compressibility cannot guarantee upper or lower bound for the real time of the process.

Note that the mentioned numerical model is the modification of the model for studying the time-dependent regimes of cooling the porous energy-release objects [16-18], which also was modified and applied for investigating the heterogeneous combustion in porous media [19-21] and was validated by means of experimental data [22]

The present work is devoted to development of numerical model of two-dimensional planar time-dependent gas flows through bed of granular PCM. Influence of heat losses through the side walls and heat conductivity of the PCM on regime of movement of mushy zone in the granular bed and on configuration of the mushy zone boundaries is investigated.

2. Description of the Numerical Model
Let us consider the motionless porous object consisting of granular PCM and bounded by the opened horizontal surfaces at the top and at the bottom and by the vertical impermeable side walls. The hot gas flows into the object at the bottom (inlet) at given pressure and temperature, flows up through the object heating the PCM particles, and flows out at the top (outlet) at a given pressure. When attaining a certain temperature, the heated PCM melts without loss of stability of the particles due to special granulation or encapsulation of the material.

The mathematical model of the described process is based on the model of heterogeneous continua mechanics [23] and includes the equations of energy for the granular PCM and the gas, the motion and continuity equations for the gas, and the equation of state of the perfect gas. In PCM energy equation, we take into account the heat conductivity of the PCM and the heat exchange between the PCM particles and the gas which is assumed to be proportional to the difference of their temperatures in the considered point of the medium. The phase change is taken into account in this equation in a form of additional term which is proportional to the rate of the liquid fraction of the PCM by the analogue with mushy zone model [8]. The gas energy equation takes into account the heat conductivity and heat exchange with PCM. The momentum conservation equation for porous media is used for describing the gas dynamics. This equation can be considered as a generalization of the Darcy's low. In works [12-15] the mentioned equation also included the inertial resistance to gas motion which is proportional to the squared velocity of gas filtration. But in the present study when investigating the regimes of mushy zone propagation in the granular bed this term can be omitted without significant loss of accuracy. It was shown in [16] that taking into account the temperature dependence of the gas dynamic viscosity at modelling time-dependent regimes of gas cooling of the porous energy-releasing elements can change the solution both quantitatively and qualitatively. When modelling the thermal energy storage based on granular PCM with gaseous heat transfer fluid, large temperature gradients can appear which can significantly change the viscous resistance and impact on the gas flows though the granular PCM. So, we will take into account the temperature dependence of the gas dynamic viscosity by the Sutherland formula. Thus, the system of equation describing two-dimensional planar time-dependent gas flows through the bed of granular PCM can be written as follows:

\[ (1-a)\rho_c c_c \frac{\partial T_c}{\partial t} = -a(T_c - T_g) \left( 1-a \right) \lambda_c \left( \frac{\partial^2 T_c}{\partial x^2} + \frac{\partial^2 T_c}{\partial y^2} \right) - (1-a) \rho_c Q \frac{\partial f}{\partial t}, \]
\[
\rho \frac{c_p}{g} \left[ a \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right] = \alpha \left( T_e - T_g \right) + a \lambda \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2},
\]

\[
1 + \frac{(1-a)/\lambda}{2} \rho \frac{u}{t} \left[ a \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right] = -\frac{\partial p}{\partial x} - \frac{\mu}{k} u,
\]

\[
1 + \frac{(1-a)/\lambda}{2} \rho \frac{v}{t} \left[ a \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right] = -\frac{\partial p}{\partial y} - \frac{\mu}{k} v - \rho \left[ g, f, \rho \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, p = \rho_g RT_g,
\]

\[
\mu = \frac{t^2}{c_1 + T_g}, f = \begin{cases} 0, & T_e < T_{ml}, \\ (0.1), & T_e = T_{ml}, \\ 1, & T_e > T_{ml}. \end{cases}
\]

where \(a\) is the porosity, \(c\) is the specific heat capacity, \(c_1\) and \(c_2\) are constants in Sutherland formula, \(f\) is the liquid fraction of the PCM, \(g\) is the acceleration of gravity, \(k\) is the coefficient of permeability of the porous medium, \(Q\) is the latent heat of the PCM, \(p\) is the gas pressure, \(R\) is the gas constant, \(T\) is the temperature, \(t\) is the time, \(u\) and \(v\) are the horizontal and vertical components of the gas filtration velocity respectively, \(x\) and \(y\) are the horizontal and vertical spatial coordinates respectively, \(\alpha\) is the constant determining the intensity of the interphase heat exchange, \(\lambda\) is the heat conductivity coefficient, \(\mu\) is the coefficient of dynamic viscosity of the gas, \(\rho\) is the density, \(\chi\) is the coefficient taking into account the inertial interaction of the media in their relative accelerated motion [23].

Indexes \(c\) denotes the PCM, \(g\) denotes the gas, \(ml\) denotes the melting point, \(p\) denotes the value at a constant pressure.

Functions \(T_c\) and \(f\) are determined from the PCM energy equation in accordance to the idea described in [12, 13]. While the temperature of the PCM is not equal to its melting point, the summand with \(f\) becomes equal to zero, and \(T_c\) is found from the equation. When the PCM temperature attains its melting point, the left side of the equation becomes equal to zero, and we determine \(f\) until it attains value 1 which corresponds to the full melting of the PCM in the considered point. The similar algorithm is applied when modelling the solidification of the PCM.

The pressure and the temperature of the gas are known in the inlet to the porous object; the gas pressure is given in the outlet. The heat transfer conditions are known at the opened and impermeable boundaries of the object. Thus, let us write the boundary conditions for the system (1) as follows:

\[
p|_{t=0} = p_0, \quad T_g|_{t=0} = T_{g0}, \quad \lambda \frac{\partial T}{\partial y}|_{t=0} = \beta \left( T_e|_{t=0} - T_{g0} \right),
\]

\[
p|_{t=H} = p_H, \quad \frac{\partial T_g}{\partial y}|_{t=H} = 0, \quad -\lambda \frac{\partial T}{\partial y}|_{t=H} = \beta \left( T_e|_{t=H} - T_g|_{t=H} \right),
\]

\[
\lambda \frac{\partial T}{\partial x}|_{t=0} = \gamma \left( T_e|_{t=L} - T_e\right), \quad \lambda \frac{\partial T}{\partial x}|_{t=L} = \gamma \left( T_e|_{t=L} - T_e|_{t=L} \right), \quad \frac{\partial T}{\partial x}|_{t=0} = \frac{\partial T_g}{\partial x}|_{t=0} = 0, \quad u|_{t=0} = u|_{t=L} = 0,
\]

where \(H\) and \(L\) are the height and the width of the porous object respectively, \(p_0, p_H\) and \(T_{g0}\) are the known values of pressure and temperature of the gas respectively, \(T_{e0}\) is the ambient temperature, \(\beta\) is the heat transfer coefficient, \(\gamma\) is the coefficient determining the intensity of heat losses through the side walls.

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

The original finite-difference algorithm is proposed to solve the system of equations (1) with boundary conditions (2). According to the algorithm, the equations of energy and motion of the gas are
transformed into the explicit finite-difference equations, which the temperature and the gas filtration velocity components are defined from. The energy equation for the PCM is also transformed into the finite-difference equation which the PCM temperature and the liquid fraction are defined from by the explicit scheme using the above-mentioned algorithm. Herewith, the possible energy losses caused by the discretization of the problem are corrected as in work [13] where the one-dimensional gas flow through the bed of granular PCM is considered. The gas continuity equation is transformed into implicit finite-difference equation as following. Denote the time layer number with known values of sought parameters as $n$ and the time layer with unknown values of the parameters as $(n + 1)$. So, the partial derivative by $x$ in the continuity equation is approximated on the $n$th time layer and the derivative by $y$ is approximated on the $(n + 1)$th layer. The gas pressure is defined from this equation by the Thomas algorithm [24] with taking into account the perfect gas equation of state. Note that the described approximation of the continuity equation allows to avoid solving the complex systems of equations and to parallel the algorithm by means of geometric decomposition. The gas density is determined from the state equation of the perfect gas.

The described numerical method was realized in one-dimensional case and was validated by means of comparison of calculation results with experimental data which is discussed in [12, 13] and shown the good coincidence of the data.

3. On Mushy Zone Motion in the Bed of Granular PCM
Since in practice the main purpose of the thermal energy storages considered in the present work is the accumulation of heat due to the latent heat of the PCM, the influence of heat losses through the side walls on the melting process of the material in the bed and on the propagation of the mushy zone is of interest. In further for usability let us denote the mushy zone boundaries which are the line separating the mushy zone from the region of the liquid PCM and the line separating the mushy zone from the region with the PCM in the solid state as $\eta_1$ and $\eta_2$ respectively. Figures 1 and 2 depicts the lines bounding the mushy zone at different moments of time for different values of the PCM heat conductivity coefficient and following values of problem parameters:

$$
a = 0.3, \ c_v = 2250 J/(kg \cdot K), \ c_{sp} = 10^7 J/(kg \cdot K), \ c_{st} = 1.458 \cdot 10^6 kg/(m \cdot s \cdot K), \ c_{s2} = 110.4 K,$$

$$
g = 9.81 m/s^2, \ k = 10^{-8} m^2, \ Q = 10^3 J/kg, \ p_0 = 1.05 \cdot 10^5 Pa, \ p_{H} = 10^5 Pa, \ R = 287 J/(kg \cdot K),$$

$$
T_{g0} = 400 K, \ T_w = 350 K, \ T_{\infty} = 300 K, \ H = 2 m, \ L = 1 m, \ \alpha = 5 \cdot 10^5 W/(m^3 \cdot K),$$

$$
\beta = \gamma = 10 W/(m^3 \cdot K), \ \lambda_g = 2.2 \cdot 10^{-2} W/(m \cdot K), \ \rho_c = 1500 kg/m^3, \ \chi = 0.5.$$

It can be seen from the both figures that mushy zone increases in size over the time during its motion from the inlet to the outlet of the porous object. We can see from the figures 1.a and 2.a that curvature of the phase change fronts is almost absent for both heat conductivity coefficients of the PCM at initial stage of the process when the mushy zone is near the bottom part of the object. Figures 1.c and 2.c demonstrate the mushy zone located near the top part of the object; in these figures the curvature of the phase change fronts caused by the heat losses is seen most clearly. We can see that uniformity of the mushy zone boundaries over the almost all width of the object is typical for the lower value of the heat conductivity coefficient in figure 1.c and sharp curvature occurs only near the side walls. The higher value of the heat conductivity coefficient in figure 2.c results in smoother curvature of the mushy zone boundaries because of faster smoothing of the PCM temperature gradients. However, if we consider the difference between maxima and minima of the vertical coordinate of the line $\eta_2$, we can see that this difference is more for the lower heat conductivity coefficient (figure 1.c) than one for higher value of the heat conductivity coefficient (figure 2.c). In other words, the higher coefficient of heat conductivity of the PCM corresponds to the less delay of the mushy zone boundaries near the side walls from those in the central part of the object. Thus, at low heat conductivity of the PCM, it melts almost uniformly at the wide part of the object, but the high heat conductivity of the PCM provides the less delay of the melting process near the side walls in relation to the central part of the object.
Figure 1. Location of (1) line $\eta_1$ and (2) line $\eta_2$ at (a) 15, (b) 50 and (c) 80 minutes after beginning of the process at $\lambda_c = 1$ W/(m·K).

Figure 2. Location of (1) line $\eta_1$ and (2) line $\eta_2$ at (a) 15, (b) 50 and (c) 80 minutes after beginning of the process at $\lambda_c = 20$ W/(m·K).
4. Conclusion
The mathematical model and numerical method are proposed for modelling the two-dimensional planar time-dependent gas flows though bed of granular PCM. The influence of heat losses through side walls on melting process of the PCM and on motion of mushy zone is investigated by means of the proposed numerical model. It is shown that intensive heat losses provide the curvature of the mushy zone boundaries and nonuniform melting of the material in the bed. Herewith, the lower heat conductivity of the PCM obtains more uniform melting of the granular PCM over the bed's width at the wide part of the object, but the higher thermal conductivity provides the less delay of the melting near the side walls in relation to the central part of the bed.

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