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MATHEMATICAL MODELS OF COUPLED HEAT TRANSFER AND HYDRODYNAMIC PROCESSES WITH PHASE TRANSITIONS IN ENERGY-SAVING TECHNOLOGIES AND ENVIRONMENTAL SAFETY

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The paper presents a comprehensive mathematical and physical model of coupled heat transfer processes and hydrodynamics suggesting melting and solidification of inhomogeneous media with due account of medium's thermal conductivity and presence of a gravity-driven moving heat source. Models are based on the application of continuous indicator-function of phases. The paper provides the results of the calculations and their comparison with experimental data and analytical solutions.

Key words: *radioactive west, self-burial, mathematical models, function-indicator of phases.*

Introduction

Intensive studies on energy accumulation technology based on reversible-phase materials and the development of high-performance heat-storage systems have been performed in recent years. To address the problems associated with the development of relevant equipment, coupled heat transfer and hydrodynamic processes should be studied accounting for a wide range of changes in the thermophysical properties of materials, operating and structural parameters given relevant phase transformations. Mathematical models of these processes and the corresponding software package are seen as the key tools enabling to address these challenges.

Similar problems arise when RW is disposed of using the self-burial method. The idea of the self-burial method is quite simple and has been known for a long time [1—6]. Capsules with RW are emplaced into a pre-drilled well. Due to heat generation, the capsules will heat and melt the surrounding rock and, under the influence of their own weight, sink deeper, displacing the generated melt. Implementation of this disposal method is associated with the following challenges. Typical size of the capsules should not be too large, since the costs associated with drilling of large diameter wells, as well as transportation of fuel capsules to the disposal site would be too high. On the other hand, if the capsules are small, the heat release intensity being dependent on the decay rate of radionuclides and the energy released during a single fission event, would be insufficient to ensure the bedrock melting [7—10].

Therefore, this article summarizes the developed complex mathematical and physical models of coupled heat transfer and hydrodynamic processes suggesting melting and solidification of inhomogeneous media with due account of medium's thermal conductivity and presence of a gravity-driven moving heat source. The developed models were

implemented in a software package. This also enabled to created a tool addressing both the problems associated with the development of efficient heat storage systems and those associated with the gravity-driven self-disposal of heat-generating RW capsules in heterogeneous geological media.

This paper presents a comparison of calculation results with relevant analytical solutions and experimental data [13, 14].

Problem definition. Basic equations

The mathematical model of the processes described above is reduced to a joint solution of non-stationary Navier-Stokes equations, the heat equation accounting for phase transformations and equation for gravity-driven motion of a distributed inhomogeneous heat source.

The mobile interphase boundary, as well as the moving heat source are considered as the main challenges in the numerical implementation of mathematical models presenting heat transfer processes. To address these challenges the following methods were proposed in this paper: "end-to-end" calculation method was suggested to identify this boundary with no iterations, as well as application of moving grids allowing to consider the heat source movements. The idea is based on the methods proposed earlier [11, 12]. Presence of a moving heat source is seen as a notable point of contrast which necessitates the use of moving grids.

Assuming the validity of Boussinesq approximation for buoyancy and that the melt is incompressible, mass and momentum conservation equations for the melt can be respectively stated for a fixed coordinate system with its origin corresponding to the mass center of the source:

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\eta \frac{\partial u_i}{\partial x_j}\right) - \frac{\partial p}{\partial x_i} + S_{mi} + S_b \delta_{2i}, \tag{2}$$

where ρ is the density, u_i is the velocity component, η is viscosity, p is pressure, δ_{2i} is the Kronecker symbol, S_{mi} is the Darcy-type source term [11]. The latter one defines the flow in the zone between the medium and the melt, considered as a porous medium, and can be described as follows:

$$S_{mi} = -C\frac{(1-\gamma)^2}{\gamma^3 + \varepsilon} u_i. \tag{3}$$

where γ stands for the melt fraction, C is a large constant specifying the permeability of the porous medium, and ε is a small number specified to avoid dividing by zero in (3) for the solid phase.

Another source term in (2) reflects the Boussinesq approximation:

$$S_b = \rho g\left[1 - \max\left(\beta(T - T_s), 0\right)\right], \tag{4}$$

where β stands for volume expansion coefficient, g is the gravity acceleration, and T_s is the temperature of the solid medium.

In terms of enthalpy, the energy conservation equation can be presented as follows:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u_j h)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) + Q, \tag{5}$$

where λ is thermal conductivity, Q is the volumetric heat release, h is the enthalpy taking into account the phase transition power and is derived based on temperature dependence:

$$h = h_s + L(T) = \int_{T_{ref}}^{T} c dT + \gamma L, \tag{6}$$

where c is the heat storage capacity, γ is the melt fraction and L is the latent heat of phase transitions. Commonly applied approach suggests that the melt fraction γ [11] can be calculated as follows:

$$\gamma = \begin{cases} 0, & T < T_S \\ \dfrac{T - T_S}{T_l - T_S}, & T_S < T < T_l \\ 1, & T > T_l \end{cases}$$

where T_S and T_l are the solidus and liquidus temperatures, respectively.

In this paper, we use the expression for γ in the form of a continuous error function.

$$\gamma = 0{,}5\,\mathrm{erf}\left(\frac{4(T - T_m)}{(T_l - T_s)}\right) + 0{,}5, \tag{7}$$

where T_m is the arithmetic mean of T_S and T_l.

Using equations (6) and (7), equation (5) can be transformed as follows:

$$\frac{\partial(\rho c T)}{\partial t} + \frac{\partial(\rho u_j c T)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) + S_h + Q, \tag{8}$$

$$S_h = -4\rho L\, A(T)\left(\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j}\right),$$

$$A(T) = \exp\left(\left(\frac{4(T - T_m)}{(T_l - T_s)}\right)^2\right)\left(\pi(T_l - T_s)\right)^{-1}. \tag{9}$$

As follows from (8) and (9), the energy equation (8) is not a function of the melt fraction, therefore, additional iterations are not required to solve it.

The motion equation for an immersed heat source can be presented as follows:

$$m\frac{dU}{dt} = F_{fr} - F_g, \qquad (10)$$

$$F_g = (\rho_s - \rho_l) gV,\ F_{fri} = \int p\delta_{ij} - \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{x_i}\right)ds,$$

where r_s, r_l are the densities of the surrounding rock and melt, respectively, $u_1 = U$ at the source-melt interface. Under the steady-state immersion process, the velocity U is constant and equation (10) transforms into $F_{fr} = F_g$.

Given relations (3), (4), (7) and (9), equations (1), (2), (8) and (10) constitute a mathematical model of the coupled heat transfer and hydrodynamic processes taking into account melting and hardening, thermal conductivity and presence of a gravity-driven moving heat source.

The proposed formulation suggests that additional iterative procedures to determine the position of the phase boundary are not needed.

Analytical solutions of these equations were derived for simple geometries using substantial simplifications [7, 10, 13, 14]. Figure 1 shows the self-burial diagram for a fuel ball or a long cylinder. Navier-Stokes equations were replaced by lubrication theory equations which stands for the basic simplification of the model applied to derive analytical solutions along with linear or parabolic approximation of the temperature profile in the melt instead of solving the heat equation. The analytical solutions were used to verify the presented model and software complex.

Numerical implementation and calculation results

Spatial discretization of the equations for the mathematical model considered is based on second-order algorithms with moving grids. Second-order implicit time algorithms were applied with PISO splitting scheme being in place. The solution algorithm is viewed as an iterative process with its completion criterion accounting for the fulfillment of the following condition: $F_{fr} = F_g$, i.e. the equality of Archimedes force and hydrodynamic forces. The corresponding software package is implemented as part of the OPENFOAM open software environment.

To test the model and verify the program, two test tasks were specified. The first problem considers the self-burial of a heat-generating sphere into the ground. This problem was solved analytically

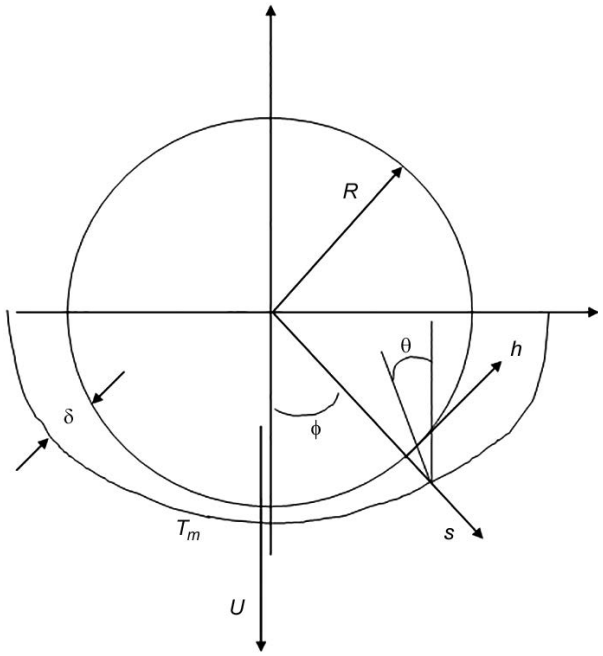

Figure 1. Self-burial diagram for a fuel ball or a long cylinder

Here: U is ball velosity, R is ball radius, T_m is melting temperature

in various approximations in [7] and [14]. The solutions obtained differ little from each other. The second test task is taken from [13] presenting the results of experimental studies on cylinder self-burial in paraffin.

Figure 2 presents the computational domain and the deformed moving mesh before stationary immersion speed was achieved under the first test. The following results were obtained from calculations of the ball's self-burial speed U given the physical properties of the ball material and surrounding ground presented in [7] [m/s]:

- according to the above model — $U_{н.р.} = 1.2e-5$,
- according to [14] — $U_{[14]} = 1.6e-5$.

A small discrepancy can be explained by the fact that the viscous friction force was not taken into account in a simplified model of the self-burial process presented in [14].

Figure 3 shows the computational domain for the test problem focused on the self-burial of a heated cylinder into paraffin and the fraction of the melt at a steady immersion rate.

To compare the calculation result with the experimental data [13], a case study was chosen suggesting that the temperature on the cylinder wall accounted for $T_w = 32$ °C, whereas the temperature in paraffin amounted to $T_\infty = 10$ °C. The thermophysical properties of the materials were taken from [13]. The calculated self-burial rate of the cylinder amounted to $U_{н.р.} = 2.8e-5$ m/s. Whereas, the experimental value obtained in [13] amounted to $U_{[13]} = 3e-5$ m/s.

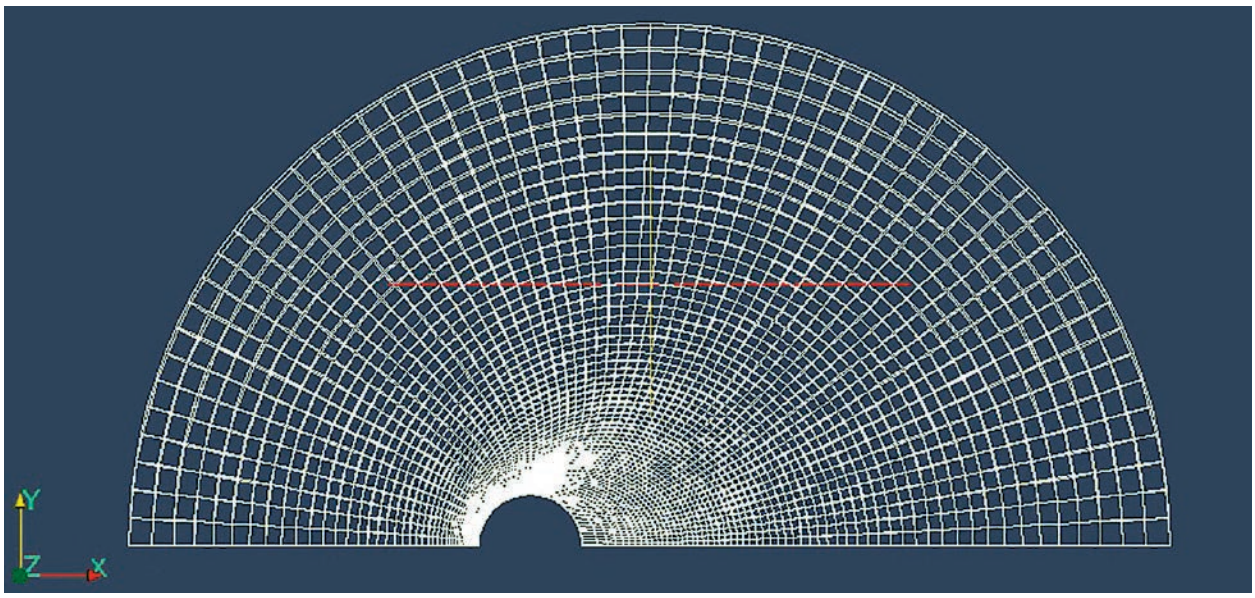

Figure 2. Computational domain and moving grid for the self-burial of a heat-emitting ball into ground

Figure 3. The magnitude of the melt velocity around the self-sinking source

It should be noted that all calculations were carried out for an unsteady self-burial process until a steady state was reached.

Conclusion

A mathematical model of coupled heat transfer and hydrodynamic processes accounting for melting and solidification, thermal conductivity and presence of a gravity-driven moving heat source was developed. "End-to-end" counting method requiring no iterations to determine the position of the phase boundary was presented. Calculations were performed with relevant comparison of the results and experimental data, as well as analytical solutions. Comparison showed their good agreement.

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