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The Conjugate Equations in the Heterogeneous Systems Heat and Mass Exchange Tasks

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Conjugate equations based on a conception of the uniform mathematic description of a naturally equal heating transfer process in all points of a heterogeneous system is proposed. The equations may be applied to describe the heat and mass exchange processes in the divided boundaries of the heterogeneous systems instead of conventional IV type boundaries conditions. The modeling results of the underground coal gasification heat and mass exchange is adduced in the new problem definition.

Keywords: heterogeneous system, divided boundaries, heat and mass exchange, type IV boundary conditions, conjugate equations, underground gasification, coal-bed reaction channel.

Introduction

The research of heat-mass exchange processes (HME) is very actual area today. The results of the researches is much used power engineering, metallurgy, chemicals, building and space exploration.

Mathematical modeling HME processes in heterogeneous systems is consider. In the systems separate phases have different physical properties and is in close contact. The systems describes by boundary conditions IV type. It's writes as equal of temperature and heat transfer rate of contact phases. The equation accuracy is heating effects in boundaries (surfaces division)

$$t_1 = t_2 = t_{\xi}; \quad \lambda_1 \frac{\partial t}{\partial n} - \lambda_2 \frac{\partial t}{\partial n} = Q(\xi, \tau, t(\xi)),$$
 (1)

1, 2 – indexes of first and second boundary contacts phases; t_1, t_2, t_ξ – temperature of first, second and third phases in the boundary, °C; λ_1, λ_2 – coefficient of heat conductivity first and second phases, W/(m·K); n – normal on division surface; ξ – point coordinate, which placed on the division surface, m; $Q(\xi, \tau, t(\xi))$ – heat effect on the division surface, W/m².

HME tasks in heterogeneous systems described IV type boundary conditions refers to conjugate tasks HME.

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1. Conjugate heat-mass exchange tasks with static and mobile division boundary

The HME tasks divides to two class conjugate tasks in dependence of specific conditions on phases division boundary. The first class is task with static boundaries, the second is task with mobile boundaries.

The tasks of first class includes tasks inside/outside convectional HME between liquid (gas) flow solid body. And besides it includes many tasks of heat-mass exchange between static bodies, e.g. solid – solid, solid – liquid and no mixed liquids [1–6].

In case of static bodies with static division boundaries in formula (1) heat effect is null and IV type boundary condition becomes simple:

$$t_1 = t_2 = t_\xi; \quad \lambda_1 \frac{\partial t}{\partial n} - \lambda_2 \frac{\partial t}{\partial n} = 0.$$
 (2)

Heterogeneous systems HME tasks with phase and chemical transformations bringing to changing divisions boundary put into the second class [7–17].

Stefan task was an early one of the second class. Historically just in Stefan task the IV type boundary condition was used for the first time in 1889. It was described wet ground freeze process wing phase transmissions of water [7]. The boundary condition with origin (drain) as hidden heat of phase transmissions write down on mobile boundary:

$$t_1 = t_2 = t_{ph}; \quad \lambda_1 \frac{\partial t}{\partial n} - \lambda_2 \frac{\partial t}{\partial n} = q_{ph} \cdot \rho \frac{d\xi}{d\tau},$$
 (3)

 t_{ph} – water phase transmission temperature (to ice and inversely), °C; q_{ph} ; ρ – specific phase transfer hidden heat of dry ground J/kg and dry ground density, kg/m³; $d\xi/d\tau$ – phase transfer boundary movement velocity, m/s.

It should be noted that in coarse-dispersed grounds the water phase transmission temperature is constant $-t_{ph}$ =const because water is in free. And water in fine-dispersed grounds is bound, so freezing occur in range of temperatures t_{ph} =var.

Tasks with state of matter changes and relating boundaries movement would refer to Stefan tasks in what follows. In this case in the systems of bodies with the phase transitions allows for heat emission in solidification zone by solution or melt phasing diagram [8–12]:

$$C_{cr}\frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left(\lambda_{cr} \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_{cr} \frac{\partial t}{\partial y} \right) + q_{cr} \rho_{cr} \frac{dS(\tau)}{d\tau}, \tag{4}$$

 C_{cr} , λ_{cr} – volumetric heat capacity, J/(m³K), and heat conductivity in solidification zone as function of coordinates and temperature; S(τ) – function of heat emission in solidification zone by state of body diagram. In the phase division boundary writes IV boundaries conditions as before (3).

In addition Stefan tasks to second class of HME mobile boundary conjugation tasks refers tasks of chemical conversions with heat emissions or absorptions in the phase division boundary [13–16]. For example it's burning and thermo chemical destruction of solid fuels wich blows high-enthalpy gas. IV type boundary condition writes for temperature fields and heat flows conjugation in phase division boundary in this case [13]:

$$t_g = t_s = t_w; \quad \lambda_g \left(\frac{\partial t}{\partial y}\right)_g - \lambda_s \left(\frac{\partial t}{\partial y}\right)_s = \sigma \varepsilon \cdot \left(T_w^4 - T_e^4\right) - \sum_{i=1}^n q_i \cdot R_{si},$$
 (5)

g, s, w, e – gas flow, solid body, phase division boundary (wall) and external surface of boundary layer indexes; y – coordinate of orthogonal system; σ , ε – Stefan–Boltzmann constant, 5,7·10⁻⁸ W/(m²K⁴), and emissivity; q_i , R_{si} – heating effect and solid boby disappearance mass velocity by i-th heterogeneous chemical reaction in the wall, kg/(m²s).

Besides condition (5) components mass-conservation conditions writes in the phase division boundary. For gas the heat exchange describes energy equation subject to homogeneous reactions heat volume sources. For solid fuel the heat exchange describes thermal conductivity equation or if the solid fuel would have porosity and so diffusion-convective thermal conduction process would be have energy equation too.

When III type boundary conditions uses to describe nonstationary HME processes in heterogeneous systems the temperature fields of the modeling system divided to independent sections. The problem statement result to improbable and inconsistent solutions [3, 8, 13]. Instead of this case IV type boundary conditions give able to consider the heterogeneous systems as single whole by consideration thermal interaction between all particles.

However a question is appear — Why the transfer of substance, for example energy, impulse, amount of the substance, in the united system modeling by different mathematical ways? In the volume of bodies the heat transfer describes by energy equation and otherwise in boundary by equation of IV type boundary condition, when the physical laws not change. May the energy or heat conductivity equations use as conjugation of volumes and boundaries of HME tasks?

2. The uniform heat transfer mathematic description in phase volume and boundaries conception

The conception was to bring forward by authors [17] and where was apply conjugation equation instead of IV type boundary condition. The conception based on the next reasoning.

Let's look flat HME task between solid body and washed liquid which have different temperature in initial time. Let's place elementary volume Δx , Δy thereby one half is on solid body and another is on washed liquid (Fig. 1). Let's call it conjugate elementary volume.

Thermophysic properties of solid body is the same by nature in conjunction volume 1'and in volume of body 1. As well washed liquid 2 and 2' is. The properties have difference by quantitatively but not qualitatively.

On the other hand thermal transfer processes is unchangeable by their nature thermal conductivity, convection and radiation regardless of place in the considered body either in volume of phase or divided boundary.

Thereby substance thermophysic properties sameness and thermal transfer processes unchangeable in the volume and in boundary implicate their identical formalized description as energy equation independently to current point place either in heterogeneous system.

2.1. The conjunction equation in fixed boundary tasks

Let's conclude differential heat transfer equation in fixed divided boundary conjunction voluentary unit (Fig. 1). Let's make next assumptions in the case:

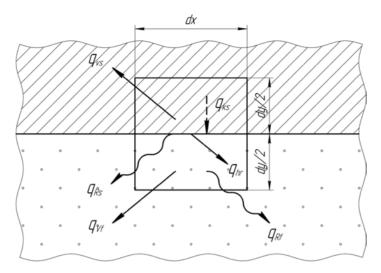


Fig. 1. The conjugate elementary volume: 1 – the fluid flow (gas mixture); 2 – the solid body; 1', 2' – fluid flow and the solid body in the conjugate elementary volume correspondently

- bodies in the conjunction unit 1' and 2' is homogenous and isomorphous;
- p = const;
- liquid is incompressible;
- liquid motion is stationary with velocity vector projection Ox, $Oy w_x = const$, $w_y = const$;
- bodies inside heat origins specify as space coordinates and time functions;
- fiction is neglect.

The interactive bodies heat quantity changing in voluentary unit through time interval $\Delta \tau$ may to define

$$\Delta Q = \Delta Q_{ht} + \Delta Q_{v},\tag{6}$$

 ΔQ_{ht} – heat quantity coming in voluentary unit $\Delta V = \Delta x \Delta y$ by heat conductivity and convection, J; ΔQ_v – heat quantity emitting in ΔV at the expense of inside heat origins, J.

Let's define first component of (6) by examine lower and upper semi-elements $\Delta V_{1/2} = \Delta x \Delta y/2$ (Fig. 1). The first body values will denote by f symbol and second – s.

In lower semi-element from liquid through Δx face in the axis Oy direction will have come a heat quality. It will $\Delta Q_y = q_y^{(f)} \Delta x \Delta \tau$ for a $\Delta \tau$. And the heat quality which will come out through opposite

face will $\Delta Q_{y+\Delta y/2} = q_{y+\Delta y/2}^{(f)} \Delta x \Delta \tau$.

Let suppose that $q_{y+\Delta y/2}^{(f)}$ function is continued on $\Delta y/2$ interval. The Taylor series of the function is

$$q_{y+\Delta y/2}^{(f)} = q_y^{(f)} + \frac{\partial q_y^{(f)}}{\partial y} \Delta y/2 + \frac{\partial^2 q_y^{(f)}}{\partial y^2} \frac{(\Delta y/2)^2}{2!} + \dots$$
 (7)

Let's take two first series terms. In the lower semi-element will collect a heat quantity by axis Oy heat flux for a $\Delta \tau$ time. The heat quantity is

$$\Delta Q_y^{(f)} = \Delta Q_y - \Delta Q_{y + \Delta y/2} = -\frac{\partial q_y^{(f)}}{\partial y} \Delta x \frac{\Delta y}{2} \Delta \tau.$$
 (8)

In much the same way a lower semi-element heat quantity by axis Ox heat flux for a $\Delta \tau$ time and a upper semi-element heat quantity by heat flux of axis Ox, Oy for the same time is

$$\Delta Q_{x}^{(f)} = -\frac{\partial q_{x}^{(f)}}{\partial x} \Delta x \frac{\Delta y}{2} \Delta \tau;$$

$$\Delta Q_{y}^{(s)} = -\frac{\partial q_{y}^{(s)}}{\partial y} \Delta x \frac{\Delta y}{2} \Delta \tau; \quad \Delta Q_{x}^{(s)} = -\frac{\partial q_{x}^{(s)}}{\partial x} \Delta x \frac{\Delta y}{2} \Delta \tau.$$
(9)

As a result of applying of (8), (9) in the lower semi-element will be

$$\Delta Q_{ht}^{(f)} = \Delta Q_x^{(f)} + \Delta Q_y^{(f)} = -\left(\frac{\partial q_x^{(f)}}{\partial x} + \frac{\partial q_y^{(f)}}{\partial y}\right) \Delta x \frac{\Delta y}{2} \Delta \tau = -div \ q^{(f)} \ \Delta x \frac{\Delta y}{2} \Delta \tau,$$

And in upper semi-element will be

$$\Delta Q_{ht}^{(s)} = -div \ q^{(s)} \ \Delta x \frac{\Delta y}{2} \Delta \tau$$
.

A total heat quantity accumulated in the conjunction elementary volume ΔV may define as

$$\Delta Q_{ht} = \Delta Q_{ht}^{(f)} + \Delta Q_{ht}^{(s)} = -\left(\operatorname{div} q^{(f)} + \operatorname{div} q^{(s)}\right) \Delta x \frac{\Delta y}{2} \Delta \tau. \tag{10}$$

Let's denote a inside heat origins powers in first and second semi-elements as $q_{vf} \mu q_{vs}$. Consequently second component of (6) is

$$\Delta Q_{\nu} = (q_{\nu f} + q_{\nu s}) \Delta x \frac{\Delta y}{2} \Delta \tau. \tag{11}$$

In the isobaric process the heat which brought to elementary volume is spent to increase enthalpy ΔH in the volume completely. In that way the (6) would change to $\Delta Q = \Delta H$. In view of $dh = c_p dt$ is to incompressible liquid, we can write

$$\Delta H = \Delta H_f + \Delta H_s = \left(c_f \rho_f \frac{\partial t}{\partial \tau} + c_p \rho_s \frac{\partial t}{\partial \tau}\right) \Delta x \frac{\Delta y}{2} \Delta \tau, \qquad (12)$$

Let's set (9) - (11) to (6)

$$c_{pf} \rho_f \frac{\partial t}{\partial \tau} + c_{ps} \rho_s \frac{\partial t}{\partial \tau} = -\left(div \, q^{(f)} + div \, q^{(s)}\right) + q_{vf} + q_{vs}. \tag{13}$$

The Ox, Oy axis projection of liquid and solid body heat flux may present as

$$q_{x}^{(f)} = -\lambda_{f} \frac{\partial t}{\partial x} + \rho_{f} w_{x} h; \quad q_{y}^{(f)} = -\lambda_{f} \frac{\partial t}{\partial y} + \rho_{f} w_{y} h;$$

$$q_{x}^{(s)} = -\lambda_{s} \frac{\partial t}{\partial x}; \qquad q_{y}^{(s)} = -\lambda_{s} \frac{\partial t}{\partial y}.$$
(14)

Let's put (14) into (13)

$$c_{pf} \rho_{f} \frac{\partial t}{\partial \tau} + c_{ps} \rho_{s} \frac{\partial t}{\partial \tau} = \left(\frac{\partial}{\partial x} \left(\lambda_{f} \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_{f} \frac{\partial t}{\partial y} \right) \right) - c_{pf} \rho_{f} \left(w_{x} \frac{\partial t}{\partial x} + w_{y} \frac{\partial t}{\partial y} \right) + \left(\frac{\partial}{\partial x} \left(\lambda_{s} \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_{s} \frac{\partial t}{\partial y} \right) \right) + q_{vf} + q_{vs} ,$$

$$(15)$$

 c_{pf} , c_{ps} – the specific heat capacity, J/(kg·K); ρ_f , ρ_s – the density, kg/m³; c_{pf} , c_{ps} , ρ_f , ρ_s , λ_f , λ_s – the thermal conductivity W/(m·K) for liquid and solid phases accordingly.

Let's transfer the convective derivative in the left part equation (15)

$$c_{pf} \rho_{f} \left(\frac{\partial t}{\partial \tau} + w_{x} \frac{\partial t}{\partial x} + w_{y} \frac{\partial t}{\partial y} \right) + c_{ps} \rho_{s} \frac{\partial t}{\partial \tau} =$$

$$= \left(\frac{\partial}{\partial x} \left(\lambda_{f} \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_{f} \frac{\partial t}{\partial y} \right) \right) + \left(\frac{\partial}{\partial x} \left(\lambda_{s} \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_{s} \frac{\partial t}{\partial y} \right) \right) + q_{vf} + q_{vs}.$$

$$(15')$$

The energy equation (15) is different from the basic energy equation which written separately for the volume of the body 1 and the volume of the body 2(Fig. 1). The equation (15) includes the heat transfer of both interactive bodies among themselves in the boundary division. Let's name the equation (15) as *interactive bodies energy conjunction equation* or more simple as *conjunction equation*.

Thus eonjunction equation (15), (15') allow to model the naturally equal processes of heat transfer in heterogeneous system by the structurally equal energy equation as in volumes of bodies as in their divided boundaries without the irregular inclusion in the form of IV type boundary condition.

Let's introduce the designation for the substantial derivative of liquid flux as $\frac{Dt}{d\tau} = \frac{\partial t}{\partial \tau} + w_x \frac{\partial t}{\partial x} + w_y \frac{\partial t}{\partial y}$

. Taking into consideration that thermalphysic properties of the both bodies is constant, the conjunction

equation may rewrite as

$$c_{f}\rho_{f}\frac{Dt}{d\tau} + c_{s}\rho_{s}\frac{\partial t}{\partial \tau} = \lambda_{f}\nabla^{2}t + \lambda_{s}\nabla^{2}t + q_{vf} + q_{vs},$$

$$\nabla^{2} = \frac{\partial^{2}t}{\partial x^{2}} + \frac{\partial^{2}t}{\partial v^{2}} \text{ is Laplace operator.}$$
(16)

In contrast to considered case (Fig. 1) an occurrence is possible when two bodies moves relative to each over. The examples is liquid – gas or two immiscible dropping liquids. In the case a additional term appears. The term describes the convectional heat transfer in boundary area in the second body which early considered as immovable. Thus the both derivative in the left side of (15) equation is substantial.

The simplest form of conjunction equation (16) would to be in case of an immovable bodies interaction with an immovable divided boundary and the absence of volume thermal sources:

$$\left(c_1 \rho_1 \frac{\partial t}{\partial \tau} - \lambda_1 \nabla^2 t\right) + \left(c_2 \rho_2 \frac{\partial t}{\partial \tau} - \lambda_2 \nabla^2 t\right) = 0.$$
(17)

In this form the conjunction equation (17) is the functional analogue of IV type boundary condition (2). There is two difference between they. Firstly the heat transfer in divided boundary and the heat transfer in inside points of bodies describes equally in formalized form. In this case they describes by heat equation. Whereas in (2) instead of the heat equation uses the boundary conditions. Secondary the nonstationarity of the temperature field in dividing boundary environment models by conjunction equation itself. Due to this the conjunction equation (17) consistently blends with the mathematical model of nonstationary heat exchange in heterogeneous system. In case of the type IV boundary conditions (2) the nonstationarity of the temperature field don't denote explicitly as well as in (3) and (5). The nonstationarity express indirectly through nonstationary heat equation which writes for the bodies inside points (4). In other words the IV type boundary conditions in nonstationary conjugate HME tasks brings the induced heat inertia in the divided boundary environment. In reality nonstationary conjugate HME processes in heterogeneous systems proceeds in continual temperature changes conditions in spatial and temporal as well in the inside bodies as in the divided boundary environment.

2.2. The conjugate equation in the floating boundary tasks

If the gas mixture stream flows around the solid body and at that the heterogeneous chemical reactions of mixture components and the solid body takes place (Fig. 2) then the terms q_{hr} is appear in equation (15). Exactly the terms q_{hr} take account the thermal effects of the chemical reactions. The material dimension of the solid body will be observed with a displacement the phases divided boundary as a result of the chemical reaction.

The conjugate equation will complicate if the solid body is porosity and is permeable for gases. The porous solid fuels is thermal decomposed under heating. The decomposed process lead to the volatile matters vaporization. Under a overpressure the volatile matters filters through the porous to the phase divides surface (Fig. 2). Thereby the convectional heat transfer q_{ks} created. Besides the thermal decomposition process is endothermic reaction with heat absorption $-q_{vs}$. And so if the HME occurs in the presences of high temperatures then in equation (15) need to input the origins heat terms. The terms would to take into account the radiation of the interphase surface $-q_{Rs}$ and the radiation of the gas $-q_{Rf}$. Then in base of the reasoning equal 2.1 item the conjugate equation in vector form may write as:

$$c_{pf}\rho_{f}\frac{Dt}{d\tau} + c_{ps}\rho_{s}\frac{\partial t}{\partial \tau} = \lambda_{f}\nabla^{2}t + \lambda_{s}\nabla^{2}t + \rho_{f}\frac{\partial t}{\partial y}\sum_{i=1}^{N}c_{pi}D_{i}\frac{\partial C_{i}}{\partial y} + q_{hr} + q_{ks} + q_{vf} + q_{vs} + q_{Rs} + q_{Rf},$$

$$(18)$$

 D_i , C_i – diffusion coefficient, m²/s and mass concentration of *i*-th component of gas mixture.

Let's give some examples of using the conjugate equation (18) which take place upon mathematical modeling of the HME process in the heterogeneous systems with the floating divided boundary.

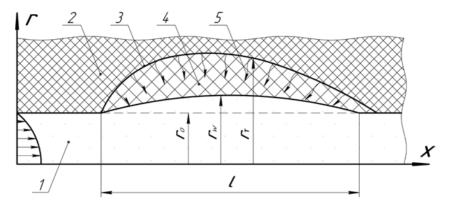


Fig. 2. The firing elaboration processes scheme of the coal-bed reaction channel: 1 – the flow of gas mixture; 2 – the peripheral layer of the coal-bed; 3 – the near-wall layer of the coal-bed which prone to the thermal decomposition; 4 – the volatile matters filtration in the coal-bed pores; ; r_0 , r_w , r_t – the radiuses of the initial channel, the mobile divided boundary of the solid body-gas and the coal thermal decomposition mobile boundary correspondently; 1 – the reaction channel length

3. The conjugate equation in the underground coal gasification HME task

In the [16] Kreinin E. V. and Shifrin E. I. produced a mathematical model wich quite complete described physical and chemical effects of the stable phase underground coal gasification (UCG) in the gas generator (GG). But strictly speaking no one of the process stages is stable. Since a moment of a fireplace creating to a reaction canal forming and further GG exploitation their material composition, a gas mixture components mass concentrations and temperature fields of the coal layer and the gas flow changes in time of the essence.

A mathematical model of a nonstationary HME reaction channel d=200 mm oxidative and reduction domains creating process in the well GG was build in the article [17] in the simplest problem definition. In the case the coal-bed is entire solid body and the only heterogeneous redox reaction C + O₂=CO₂; C + CO₂=2CO takes place in a reaction channel wall in the oxidative and reduction domains:

$$c_f \rho_f \frac{Dt}{d\tau} + c_s \rho_s \frac{\partial t}{\partial \tau} = \lambda_f \nabla^2 t + \lambda_s \nabla^2 t \pm q_k k_{ok} \exp\left(-\frac{E_k}{RT}\right) \frac{\partial C_k}{\partial r}, \tag{19}$$

 q_k , k_{ok} , E_k – thermal effect, J/mol, preexponential efficient, m/s, activation energy, J/mol, k-th heterogeneous reaction; $k = \overline{1, 2}$, $1 - O_2$, $2 - CO_2$; R – the gas constant, J/(mol·K); C_k – k-th component molar concentration, mol/m³.

In the problem definition the last term of equation (19) define a two heterogeneous reactions heat effect intensity with O₂, CO₂ components. The first occurs with calorification in oxidative domain and the second occurs with the thermal absorption in reduction domain of the reaction channel. And at the same time the wall of the channel burns down under heterogeneous reaction exposure. A reaction channel cavity enlarges by degrees. Primarily the cylindrical cavity is transformed to spindle-shaped.

The task is solved by the numerical implicit finite difference sweep method. This allowed to build the optimal algorithm by a time step variation in the condition of an essential temporal discontinuity. For example most intensive temperature field forming in the channel and the coal-bed occurs for first 24 hours. The time step was accepted as one hour for the time span. After first 24 hours the time step was increased to 24 hours by degrees.

A mathematical model offered in the articles [18] is more sophisticated then [17] one. The model takes into account an endothermic process of the coal thermal decomposition in the coal-bed body. Coal is structural changed by the thermal decomposition wich bring to coke, pitch and a volatile matters generation. The volatile matters filters through the coal-bed clefts and pours in the reaction channel (Fig. 2). In this connection in the problem definition new floating boundary appears. This is a coal thermal decomposition boundary. With all this the coal-bed is considered as a double layer system wich consists from a peripheral layer and a near-wall layer (Fig. 2). The heat transfer in the peripheral layer is described by the heat equation as before. The coal thermolysis occurs in the near-wall layer and the heat transfer there is described by the energy equation with a consideration of a convective heat transfer by the filtering volatile matters flow in the coal-bed porous space and a coal thermolysis heat origin:

$$\sum_{i=1}^{4} \varphi_{i} c_{i} \rho_{i} \frac{\partial t}{\partial \tau} + \varphi_{3} c_{3} \rho_{3} v \frac{\partial t}{\partial r} = \frac{\partial}{\partial x} \left(\sum_{i=1}^{4} \varphi_{i} \lambda_{i} \frac{\partial t}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\sum_{i=1}^{4} \varphi_{i} \lambda_{i} r \frac{\partial t}{\partial r} \right) + q_{th} \rho_{1} \frac{\partial \varphi_{1}}{\partial \tau}. \tag{20}$$

 φ_i – the *i*-th coal component in the share units: 1 –, 2 – pitch, 3 – the volatile matters, 4 – a mineral share; λ_i – the *i*-th coal component thermal conductivity; q_{th} – heat of the coal thermal decomposition, J/kg; ρ_1 – a density of the combustible share of coal in solid phase; ν – radial component of a velocity vector of a filtration the volatile matters in the coal-bed, m/s.

In the channel wall an energy conjugation equation is

$$\begin{split} &\sum_{j=1}^{7} C_{j} c_{pj} \rho_{j} \frac{Dt}{d\tau} + \sum_{i=1}^{4} \varphi_{i} c_{i} \rho_{i} \frac{\partial t}{\partial \tau} + \varphi_{3} c_{3} \rho_{3} v \frac{\partial t}{\partial r} = \frac{\partial}{\partial x} \left(\sum_{j=1}^{7} C_{j} \lambda_{j} \frac{\partial t}{\partial x} \right) + \\ &+ \frac{\partial}{\partial r_{w}} \left(\sum_{j=1}^{7} C_{j} \lambda_{j} r_{w} \frac{\partial t}{\partial r} \right) + \frac{\partial}{\partial x} \left(\sum_{i=1}^{4} \varphi_{i} \lambda_{i} \frac{\partial t}{\partial x} \right) + \frac{1}{r_{w}} \frac{\partial}{\partial r} \left(\sum_{i=1}^{4} \varphi_{i} \lambda_{i} r_{w} \frac{\partial t}{\partial r} \right) + \\ &+ q_{th} \rho_{1} \frac{\partial \varphi_{1}}{\partial \tau} + q_{3} k_{03} \exp \left(-\frac{E_{3}}{RT} \right) \frac{\partial \rho_{3} \varphi_{3} / M_{3}}{\partial r} \pm q_{k} k_{ok} \exp \left(-\frac{E_{k}}{RT} \right) \frac{\partial C_{k}}{\partial r} , \end{split}$$

 q_3 , k_{o3} , E_3 , – thermal effect, J/mol, preexponential efficient and energy of a volatile matters burning activation; M_3 – a volatile matters molecular mass, kg/mol.

In comparison of (17) the equation (19) has terms which allows coal decomposition heat in the upper semielement of a conjugate elementary volume and volatile matters burning heat in the lower semielement. It is fifth and sixth terms in right side of the equation.

In the [18] problem definition a radiation components of the energy transmission q_{Rs} , q_{Rf} did't consider by supposition that the process proceeds in well walls self-irradiation condition. And also a coal properties changing supposes quasistationary on account of slower coal-bed heating. In every new time step thermalphysics properties values recalculates by empiric formulas. For example an equivalent coal thermal conductivity factor is calculated by Roussel formula [19]:

$$\lambda_{eq} = \lambda_0 \frac{m^{2/3} + (\lambda_0 / \lambda_g)(1 - m^{2/3})}{m^{2/3} - m + (\lambda_0 / \lambda_g)(1 - m^{2/3} + m)},$$
(22)

 λ_0 , λ_g – veritable coal thermal conductivity and gas thermal conductivity factors, W/(m·K); m – coal porosity. A temperature dependence of effective heat capacity factor of Irsha-Borodino deposit on the materials [19] is approximated as:

$$c(t)_{eff} = \begin{cases} 1,05 + 0,0034t, & 0 \le t \le 200; \\ 1,68, & 200 < t \le 560; \\ 1,68 - 0,004(t - 560), & 560 < t \le 900; \\ 0,28, & t > 900^{\circ}C. \end{cases}$$
(23)

Kinetic coal description is supposed in accordance with data offering in [20].

A pitch share which generated by the coal decomposition defines from continuity equation on the analogy of [13]:

$$\frac{\partial \varphi_2}{\partial \tau} = \frac{M_2}{M_1} \frac{\rho_1}{\rho_2} \varphi_1 k_{01} \exp\left(\frac{E_{th}}{RT}\right).$$

A volatile matters share defines under the assumption of the mineral share is constant ϕ_4 = const:

$$\varphi_3 = 1 - (\varphi_1 + \varphi_2 + \varphi_4).$$

The mathematical model besides the temperature fields conjugate equation includes concentration fields conjugate equations of the gas components which simultaneously presents in the solid body and the gas mixture of channel. The concentration fields conjugate equations is similar to temperature fields conjugate equation by they structure and so don't bring here.

A computing experiment of an HME of firing well creating process with account of coal thermal decomposition had realized for the same conditions as in [17]. In the brown coal-bed from the Irsha-Borodino deposit had bored a well with the diameter 200 mm and the length 100 m. In a distance 41 m from the well entry had created a fireplace by 4 m length and simultaneous oxygen-containing blowing supply.

The results of the experiment has showed the mathematical model of an HME of firing well creating process in coal-bed with using the energy conjugate equations (21) and the diffusion conjugate equation truly adjust with physical representation of the processes nature.

For example the blowing velocity value influences deeply on the reaction channel wall temperature status and on the expansion velocity of the reaction domain front along the well axis. A essential channel wall convectional cooling on the scope of the combustion zone 41– 45 m is observed by changing the middle blowing velocity w_0 from 0,1 to 0,5 m/s (Fig. 3). With middle blowing velocity w_0 =0,06 m/s to twentieth hour from the combustion zone creating the wall temperature is higher then the initial temperature (t_0 =1000°C, dotted line 1 Fig. 3) everywhere and achieves 1220°C. The blowing velocity increasing brings to enlargement of the setback temperature domain ($t < t_0$). And when the blowing velocity reaches w_0 =0,5 m/s the wall temperature becomes lower than 1000°C along the whole length of the combustion zone (Fig. 3). A beginning section of the combustion domain is cooled to the utmost. If the blowing velocity w_0 is 0,1 and 0,3 m/s the temperature of the beginning section of the combustion domain will fall from t_0 =1000°C to 750 and 305°C correspondently. And if the w_0 is 0,5 m/s the temperature will become lower ignition point $t < t_{ig}$ =200°C (Fig. 3).

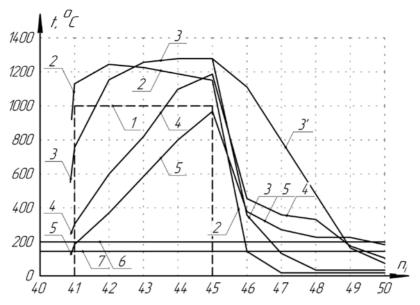


Fig. 3. The reaction channel wall temperature status on 20 th hour of the firing elaboration: 1 – the initial wall temperature; 2 – the wall temperature when blowing velocity $w_0 = 0.06$ m/s; 3 – the wall temperature when blowing velocity $w_0 = 0.10$ m/s and with taking into account the volatile matters filtration in the pores of the near-wall layer; 3' – the same without account of the volatile matters filtration; 4 – the wall temperature when blowing velocity $w_0 = 0.30$ m/s; 5 – the wall temperature when blowing velocity $w_0 = 0.50$ m/s; 6 – the coal ignition temperature; 7 – the coal thermal decomposition temperature

From the other hand blowing velocity increasing brings to increasing combustion domain front velocity along the stream. The wall temperature is distinctly increased after twenty hours of firing elaboration with w_0 =0,06 m/s. But the combustion domain length l_r had stays the same 4 m (from 41to 45 m). When w_{cp} becomes 0,3 m/s the combustion domain length becomes l_r =8 m and the front of ignition moves along to stream from 45 m point to 49 m (Fig. 3). The front of ignition moving the utmost is when the w_0 =0,5 m/s and the front achieve 49,5 m point. But on the velocity the first combustion point fades as noted above.

Besides the blast velocity the reaction channel forming is influenced by oxygen concentration on the blast. The oxygen-enriched blast C_0 =0,3-0,4 supply more intense coke burning on the channel wall and increasing the wall temperature (Fig. 3). This provides coal-bed heating and more deep combustion front moving along stream in compare an ordinary air blowing.

A preliminary blast heating 20 to 300°C before blowing it to well don't influence to reaction channel forming because the blowing has relatively low thermal capacity. The capacity is less than coal-bed thermal capacity in three times. When blowing air has passed a distance from well entry to fireplace (it's 40 m in the case) it would cooled by heat transfer with well walls. So there is no difference between lower and high temperature blowing.

The feature of the mathematical model [18] is to take into account the processes of the coal thermal decomposition in the bed and the volatile matters filtering (20) passes in the opposite direction to the coal-bed heating direction. As a consequence of this the coal-bed heating in the model is more slowly than in the model [17]. For example in the case w_0 =0,1 m/s and taking into account the coal

thermolysis and the volatile matters filtering the wall temperature in the combustion domain 3 is less in three-five times than in the model which don't consider the process 3' (Fig. 3).

Conclusions

- 1. The energy (thermal conductivity) conjugate equation was received. It bases on the conception of the uniform mathematic description of a naturally equal heating transfer process in all points of a heterogeneous system.
- 2. The energy conjugate equation on the divided boundary describes processes of the both interacting bodies. The bodies may be in different states of matter and be mobile relative to each other.
- 3. In the non-stationary HME processes the IV type boundary conditions obviously reflect only the process temporal homogeneity but the thermal inertia in points of the divided boundaries they includes only by artificially (unnaturally). In the other hand the conjugate equations equally describes the energy transfer essence in all points of heterogeneous system. And besides the conjugate equations reproduces temporal changeability of temperature and the thermal flows in an explicit form.
- 4. For appropriate describes of HME processes in heterogeneous systems isn't enough to use only temperature fields conjugate equations. Because besides heat exchange processes in the systems there is mass exchange processes with interpenetration. Therefore there is need to add the components concentration fields conjugate equations in the equation set.
- 5. The conception of the uniform mathematic description of HME process in the heterogeneous systems may apply to the underground coal gasification task. The numerical experiment results is well conform with physical representation of the reaction channel firing elaboration processes in the coalbed.

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Уравнения сопряжения в задачах тепломассообмена гетерогенных систем

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Предложены уравнения сопряжения, основанные на концепции единообразного формализованного представления одинаковых по своей природе механизмов переноса теплоты во всех точках гетерогенной системы. Уравнения сопряжения могут быть применены при описании процессов тепломассообмена на границах раздела фаз гетерогенных систем вместо традиционных граничных условий четвертого рода. Приведены результаты моделирования задачи тепломассообмена при подземной газификации угля в постановке с использованием уравнений сопряжения.

Kлючевые слова: гетерогенная система, границы раздела, тепломассообмен, граничные условия IV рода (ΓV IV рода), уравнения сопряжения, подземная газификация угля, реакционный канал угольного пласта.