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Mathematical Models of Heat Ignition And Explosion Considering Local Non-Equilibrium of Processes

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Abstract. By using the heat balance equation and the modified Fourier's law formula, where the heat flux relaxation and temperature gradient were considered, the model of heat ignition non-equilibrium process for the plate with non-linear (exponentially changing depending on the temperature) inner heat source was developed. The studies performed at relaxed boundary third-class conditions have shown that consideration of non-locality results in the increased heat ignition time irrespective of the intensity of heat exchange with the ambient medium. This fact is explained by the resistance caused by the ambient medium, the process of change of its temperature condition which increases as the relaxation factors rise. It is also shown that with consideration of the relaxation phenomena boundary conditions of the first, second and third class may not be met immediately – they may be set only within a particular range of the initial time segment. This means that the immediate implementation of the thermal impact condition seems to be impossible, since the value of heat-transfer factor has a definite limit, which depends on the relaxation properties of the medium, which may not be exceeded under any conditions of heat exchange with the ambient medium.

1. Introduction

Known heat ignition models are based on thermal conductivity parabolic equation received without considering the relaxation phenomena [1, 2]. When using them, consequently, they have an embedded heat propagation velocity, which is caused by the use the Fourier's law formula while deriving them, where the temperature gradient (the reason is driving force) and heat flow (consequence) are not time-separated. Consequently, any change of the reason causes instant change of the result. Since in actual processes, no infinite values of any parameters may occur, the equations derived based on the Fourier's law formula may be adequate to them only within a particular time range. It is known that the parabolic equations provide an inadequate description to all fast processes, whose changing time is comparable with the relaxation time as well as change of temperature at small and extrasmall values of time under any heat processes [3, 4]. Considering that during heat ignition, its delay time is determined, which is counted from the initiation of the thermal process, failure to consider non-locality in mathematical models may result in a considerable discrepancy between the results obtained and actual physical processes.

2. Mathematical task setting

To derive the differential heat ignition process considering the local no-equilibrium, let's represent the Fourier's law formula in the form of $q = -\lambda \partial T / \partial x$ [5, 6]

$$q = -\lambda\left(\frac{\partial T}{\partial x} + \tau_1 \frac{\partial^2 T}{\partial x \partial t}\right) - \tau_1 \frac{\partial q}{\partial t} \tag{1}$$

where q – heat flow; T – temperature; x – coordinate; t – time; λ – heat conductivity factor; τ_1 – relaxation factor.

By substituting (1) in the heat balance equation

$$c\rho \partial T / \partial t + \partial q / \partial x + \omega(T) = 0 \tag{2}$$

We find

$$c\rho \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} + \lambda\tau_1 \frac{\partial^3 T}{\partial x^2 \partial t} + \tau_1 \frac{\partial}{\partial t}\left(\frac{\partial q}{\partial x}\right) + \omega(T) \tag{3}$$

where $\omega(T) = Q\rho k_0 \exp(-E/(RT))$ – power of inner heat source; Q – reaction heat effect; ρ – density; c – heat capacity; k_0 – preexponential factor ; E – activation energy; R – universal gas constant.

By expressing $\partial q / \partial x$ from (2) and substituting in (3), we obtain

$$\frac{\partial T}{\partial t} + \tau_1 \frac{\partial^2 T}{\partial t^2} = a\left(\frac{\partial^2 T}{\partial x^2} + \tau_1 \frac{\partial^3 T}{\partial x^2 \partial t}\right) - \frac{\gamma}{T^2} \exp\left(-\frac{E}{RT}\right)\frac{\partial T}{\partial t} + \frac{Qk_0}{c}\exp\left(-\frac{E}{RT}\right) \tag{4}$$

where $\gamma = \tau_1 Q k_0 E/(cR)$ – a complex with the dimension K^2; $a = \lambda/(c\rho)$ – temperature conductivity. It is obvious that at $\tau_1 = 0$ the equation (4) is reduced to the parabolic heat conductivity equation with a non-linear heat source.

Let's find a solution to the equation (4) with the following boundary conditions

$$T(x,\, 0) = T_0 \tag{5}$$

$$\partial T(x,\, 0) / \partial t = 0 \tag{6}$$

$$\lambda \frac{\partial T(0,t)}{\partial x} + \lambda\tau_1 \frac{\partial^2 T(0,t)}{\partial x \partial t} = \alpha_1 [T(0,t) - T_{\mathrm{w}1}] + \alpha_1 \tau_1 \frac{\partial T(0,t)}{\partial t} \tag{7}$$

$$\lambda \frac{\partial T(\delta,t)}{\partial x} + \lambda\tau_1 \frac{\partial^2 T(\delta,t)}{\partial x \partial t} = \alpha_2 [T_{\mathrm{w}2} - T(\delta,t)] - \alpha_2 \tau_1 \frac{\partial T(\delta,t)}{\partial t} \tag{8}$$

where T_0 – initial temperature; $T_{\mathrm{w}1}$, $T_{\mathrm{w}2}$ – temperature of media; δ – plate thickness; α_1, α_2 – heat-transfer factors.

Let's introduce the following non-dimensional parameters and variables:

$$\Theta = \frac{T - T_0}{\Delta T};\quad \mathrm{Fo} = \frac{at}{\delta^2};\quad \xi = \frac{x}{\delta};\quad \mathrm{Fo}_1 = \frac{a\tau_1}{\delta^2};\quad \tau = \frac{\delta^2 Q k_0}{ca\Delta T};\quad \mathrm{Bi}_1 = \frac{\alpha_1 \delta}{\lambda};\quad \mathrm{Bi}_2 = \frac{\alpha_2 \delta}{\lambda}$$

where Θ, Fo, ξ – respectively, non-dimensional temperature, time, coordinate; τ – non-dimensional parameter; Fo_1 – non-dimensional relaxation factor; $\Delta T = T_{\mathrm{w}1} - T_0$.

Considering the adopted definitions, the task (4) - (8) will be

$$\frac{\partial \Theta}{\partial \mathrm{Fo}} + \mathrm{Fo}_1 \frac{\partial^2 \Theta}{\partial \mathrm{Fo}^2} = \frac{\partial^2 \Theta}{\partial \xi^2} + \mathrm{Fo}_1 \frac{\partial^3 \Theta}{\partial \xi^2 \partial \mathrm{Fo}} - \frac{\gamma}{(\Theta \Delta T + T_0)^2} \exp\left(-\frac{E}{R(\Theta \Delta T + T_0)}\right)\frac{\partial \Theta}{\partial \mathrm{Fo}} +$$

$$+ \tau \exp\left(-\frac{E}{R(\Theta \Delta T + T_0)}\right) \quad (\mathrm{Fo} > 0;\, 0 < \xi < 1)$$

$$\Theta(\xi, 0) = 1, \quad \partial \Theta(\xi, 0)/\partial \mathrm{Fo} = 0$$

$$\left[\frac{\partial \Theta}{\partial \xi} + \mathrm{Fo}_1 \frac{\partial^2 \Theta}{\partial \xi \partial \mathrm{Fo}} - \mathrm{Bi}_1\left(\Theta + \mathrm{Fo}_1 \frac{\partial \Theta}{\partial \mathrm{Fo}} + \Delta T_1\right)\right]_{\xi=0} = 0$$

$$\left[\frac{\partial \Theta}{\partial \xi} + \mathrm{Fo}_1 \frac{\partial^2 \Theta}{\partial \xi \partial \mathrm{Fo}} - \mathrm{Bi}_2\left(\Delta T_2 - \Theta - \mathrm{Fo}_1 \frac{\partial \Theta}{\partial \mathrm{Fo}}\right)\right]_{\xi=1} = 0$$

where $\Delta T_1 = (T_0 - T_{\mathrm{w}1})/\Delta T$; $\Delta T_2 = (T_{\mathrm{w}2} - T_0)/\Delta T$.

3. Solution by numerical method

By using the evident differential operator approximation pattern, the task (9) may be represented as

$$\left[1+\frac{\gamma}{(\Theta_k^i\Delta T+T_0)^2}\exp\left(-\frac{E}{R(\Theta_k^i\Delta T+T_0)}\right)\right]\frac{\Theta_k^i-\Theta_k^{i-1}}{\Delta\mathrm{Fo}}+\mathrm{Fo}_1\frac{\Theta_k^{i+1}-2\Theta_k^i+\Theta_k^{i-1}}{\Delta\mathrm{Fo}^2}=$$

$$=\frac{\Theta_{k-1}^i-2\Theta_k^i+\Theta_{k+1}^i}{\Delta\xi^2}+\mathrm{Fo}_1\frac{\Theta_{k-1}^i-2\Theta_k^i+\Theta_{k+1}^i-\Theta_{k-1}^{i-1}+2\Theta_k^{i-1}-\Theta_{k+1}^{i-1}}{\Delta\mathrm{Fo}\Delta\xi^2}+$$

$$+\tau\exp\left(-\frac{E}{R(\Theta_k^i\Delta T+T_0)}\right),\quad \Theta_k^0=0,\quad (\Theta_k^1-\Theta_k^0)/\Delta\mathrm{Fo}=0$$

$$\frac{\Theta_1^i-\Theta_0^i}{\Delta\xi}+\mathrm{Fo}_1\frac{\Theta_1^{i+1}-\Theta_0^{i+1}-\Theta_1^i+\Theta_0^i}{\Delta\mathrm{Fo}\Delta\xi}-\mathrm{Bi}_1\left(\Theta_0^i+\mathrm{Fo}_1\frac{\Theta_0^{i+1}-\Theta_0^i}{\Delta\mathrm{Fo}}+\Delta T_1\right)=0$$

$$\frac{\Theta_K^i-\Theta_{k-1}^i}{\Delta\xi}+\mathrm{Fo}_1\frac{\Theta_k^{i+1}-\Theta_{k-1}^{i+1}-\Theta_k^i+\Theta_{k-1}^i}{\Delta\mathrm{Fo}\Delta\xi}-\mathrm{Bi}_2\left(\Delta T_2-\Theta_{k-1}^i-\mathrm{Fo}_1\frac{\Theta_{k-1}^{i+1}-\Theta_{k-1}^i}{\Delta\mathrm{Fo}}\right)=0$$

4. Discussion of results

The calculation results of task (10) are given in fig. 1-3. If follows from their analysis that $\mathrm{Bi}_1=5$, $\mathrm{Bi}_2=10$ non-restricted temperature rise (heat ignition) does not occur and a stationary condition is observed with $\mathrm{Fo}\geq 1$ at which the heat input from the source is compensated by heat removal to the ambient medium (dashed line in fig. 1, see also fig. 3).

With $\mathrm{Bi}_1=5$, $\mathrm{Bi}_2=1$ heat ignition occurs under any Fo_1, and its delay time greatly depends on their value Fo_1 (see fig. 1, 2). Thus with the increase of Fo_1 from $2\cdot 10^{-3}$ to the value of $0{,}15$ the delay time of heat ignition in the point $\xi=0{,}9$ increases almost twice (fig. 1). The reason of delay is caused by the fact that when considering the relaxation phenomena, heat flows at boundaries increase from zero to values determined by the third-class boundary conditions for some time range. Therefore, when considering relaxation properties of the material, boundary conditions, irrespective of their type, may be met only after some initial time range $0\leq\mathrm{Fo}\leq\mathrm{Fo}^*$, where Fo^* is the time at which the set boundary conditions start to be fulfilled. Consequently, at the initial time segment, plate heating occurs under conditions of limited heat exchange with the ambient medium (at $T_{c1}>T_0$; $T_{c2}>T_0$), thus resulting in the heat ignition delay. As the relaxation factor increases irrespectively from the heating or cooling of the structure, ignition delay time rises including the case of its full heat isolation.

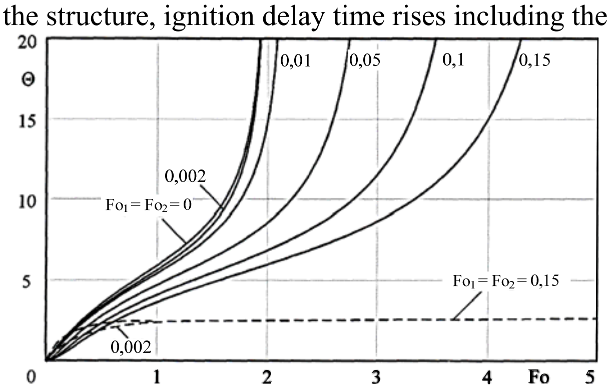

Fig. 1 Temperature history ($\xi=0{,}9$): ——— $\mathrm{Bi}_1=5$; $\mathrm{Bi}_2=5$; – – – $\mathrm{Bi}_1=5$; $\mathrm{Bi}_2=10$

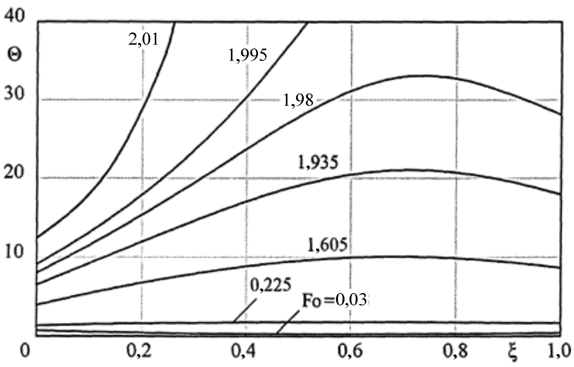

Fig. 2 Temperature change by coordinate ξ over time $\mathrm{Fo}_1=\mathrm{Fo}_2=0{,}002$; $\mathrm{Bi}_1=5$; $\mathrm{Bi}_2=1$; $\gamma=9{,}3\cdot 10^{10}$

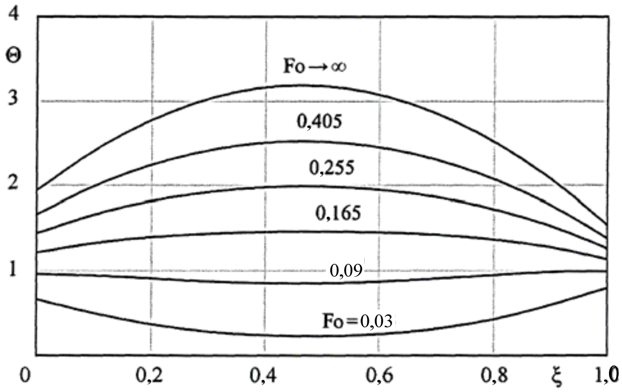

Fig. 3 Temperature change by coordinate ξ over time $Fo_1 = Fo_2 = 0{,}002$; $Bi_1 = 5$; $Bi_2 = 10$; $\gamma = 9{,}3 \cdot 10^{10}$

5. Conclusions

1. Considering the time acceleration of the heat flow and temperature gradient in the Fourier's law formula, a mathematical model of heat ignition for the plate with non-linear (exponentially depending on the temperature) heat source under the first- and third-class boundary conditions considering the time-spatial non-locality was developed.
2. Numerical studies of the model obtained have demonstrated a considerable dependence of the heat ignition delay time on the relaxation properties of materials. This fact is explained by the reason that due to the heat retention of the materials a heat flow on the wall increases from zero at the initial moment of time to the value set by the boundary condition of the first (or third) class, for some finite time interval. Consequently, heat-transfer factors may not exceed some limiting values, which depend on the thermal-physical (inclduing relaxation) properties of the body, under none conditions of heat exchange with the external medium.
3. It was shown that irrespective of the body heating or cooling, with consideration of the relaxation properties of materials, the delay time of heat ignition increases. It also increases with the absence of heat exchange at the boundaries that is when the temperature field is only determined by the effect of the inner heat source. Increasing relaxation factors would result in the extended heat ignition delay time.

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