# METHOD OF BILATERAL APPROXIMATIONS IN THE SOLUTION OF CERTAIN NONLINEAR CONSTRAINT PROBLEMS

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The solution of nonlinear constraint problems in the theory of heterogeneous ignition and heat conduction reduces to the solution of a system of nonlinear Volterra integral equations, followed by a numerical evaluation the algorithm for which is based on the use of sums analogous to Darbu sums.

The idea of successively constructing upper and lower approximating functions for an effective solution of differential equations was first proposed by Chaplygin [1]. Recently the method of bilateral approximations for solving differential equations has been developed further [2, 3]. In [3, 4] is given a method of successively constructing "upper" and "lower" approximations for solving one particular nonlinear constraint problem. We propose here an algorithm for constructing "upper" and "lower" approximations which is based on the use of sums analogous to Darbu sums.

1. Let at the instant $t = 0$ the semiinfinite space ($x < 0$) filled with a hot combustible adjoin the semiinfinite space ($x > 0$) filled with an oxidizer. The initial temperature of the combustible is $T_2^0$ and that of the oxidizer is $T_1^0$. A constant thermal flux emanates from the region $x > 0$ to the interface between the two media. We assume that the thermophysical properties are constant, that the reacting gas is an efficient binary mixture, and that at the interface there occurs a heterogeneous chemical reaction whose rate follows the Arrhenius law.

Our problem will be to determine the ignition time as a function of the initial state and of the thermokinetic properties of the reacting system.

The mathematical problem here reduces to solving the equations of heat conduction for the combustible and for the oxidizer, and the equation of diffusion for the oxidizer – all expressed in dimensionless form as

$$\frac{\partial\theta_1}{\partial\tau} = \frac{\partial^2\theta_1}{\partial y^2}, \quad y>0, \tag{1}$$

$$\frac{\partial\theta_2}{\partial\tau} = \frac{\varkappa_2}{\varkappa_1}\cdot\frac{\partial^2\theta_2}{\partial y^2}, \quad y<0, \tag{2}$$

$$\frac{\partial c}{\partial\tau} = L\frac{\partial^2 c}{\partial y^2}, \quad y>0 \tag{3}$$

with the initial and the boundary conditions

$$\theta_1|_{y=\infty} = \theta_1|_{\tau=0} = \theta_1^0, \qquad \theta_2|_{y=-\infty} = \theta_2|_{\tau=0} = \theta_2^0, \tag{4}$$

$$\theta_1|_{y=0} = \theta_2|_{y=0}, \quad \left(\omega\frac{\partial\theta_2}{\partial y} - \frac{\partial\theta_1}{\partial y}\right)_{y=0} = \alpha + c_0^n\exp\frac{\theta_0}{1+\beta\theta_0}, \tag{5}$$

$$c|_{y=\infty} = c|_{\tau=0} = 1, \quad \left.\frac{\partial c}{\partial y}\right|_{y=0} = \frac{\gamma}{L}c_0^n\exp\frac{\theta_0}{1+\beta\theta_0}. \tag{6}$$

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With the introduction of dimensionless variables, the initial temperature at the interface $T_*$ has been selected as the characteristic temperature and, by virtue of this choice, $\theta_2^0 = -\theta_1^0/K_\varepsilon$.

We note that there also occurs a heat transfer by diffusion of the reaction products and the oxidizer. According to the estimates in [5], however, this heat transfer is negligibly smaller than the heat transfer by conduction.

2. Applying the Laplace transformation [6] to the constraint problem (1)-(6), we obtain the transforms $\bar{\theta}_1(p, y)$, $\bar{\theta}_2(p, y)$, $\bar{c}(p, y)$. Inasmuch as ignition actually occurs at the interface between the two media, so for an analysis of the ignition mechanism it is sufficient to know the temperature $\theta_0(\tau)$ and the concentration of the active gas component $c_0(\tau)$ at this interface.

With the aid of the convolution theorem [6], we obtain – as the authors of [7] did – a system of nonlinear Volterra integral equations for $\theta_0$ and $c_0$:

$$\theta_0 = \frac{2}{\sqrt{\pi}\,(1+K_\varepsilon)}\left[\alpha\sqrt{\tau} + \frac{1}{2}\int_0^\tau \frac{c_0^n(t)\exp\dfrac{\theta_0(t)}{1+\beta\theta_0(t)}}{\sqrt{\tau-t}}\,dt\right], \tag{7}$$

$$c_0 = 1 - \frac{a}{\sqrt{\pi}}\int_0^\tau \frac{c_0^n(t)\exp\dfrac{\theta_0(t)}{1+\beta\theta_0(t)}}{\sqrt{\tau-t}}\,dt. \tag{8}$$

Having found $\theta_0$ and $c_0$, one can determine $\theta(y, \tau)$ and $c(y, \tau)$. For this we need the source intensity $c_0^n \exp[\theta/(1+\beta\theta_0)]$, with which $\theta(y, \tau)$ and $c(y, \tau)$ are obtained by well-known formulas [6].

It follows from Eq. (7) and (8) that

$$c_0(\tau) = 1 - a\left[(1+K_\varepsilon)\,\theta_0(\tau) - 2\alpha\sqrt{\frac{\tau}{\pi}}\right]. \tag{9}$$

System (7)-(8) then reduces to the solution of one nonlinear Volterra equation:

$$\theta_0 = \frac{2}{\sqrt{\pi}\,(1+K_\varepsilon)}\left[\alpha\sqrt{\tau} + \frac{1}{2}\int_0^\tau \frac{\varphi(\theta_0, t)}{\sqrt{\tau-t}}\,dt\right],$$
$$\varphi(\theta_0, t) = \left\{1 - a\left[(1+K_\varepsilon)\,\theta_0 - 2\alpha\sqrt{\frac{\tau}{\pi}}\right]\right\}^n \exp\frac{\theta_0}{1+\beta\theta_0}. \tag{10}$$

Two kinds of graphs of function $\varphi(\theta_0)$ are shown in Fig. 1 for $\alpha = 0$. It is easy to see that this function passes through a maximum (curve 1) at

$$\theta_0 = \theta^* = \frac{\sqrt{1 + 4n\beta + \dfrac{4n\beta^2}{a(1+K_\varepsilon)}} - 2n\beta - 1}{2n\beta^2}. \tag{11}$$

The maximum $\varphi$ will occur at $\theta_0 = 0$, if

$$a = a_0 = \frac{1}{n(1+K_\varepsilon)}. \tag{12}$$

When $a > a_0$, then the curve $\varphi(\theta_0)$ has no maximum (curve 2). A similar situation prevails when $\alpha \neq 0$.

Function $\varphi$ can be approximated by two step functions, one everywhere larger than $\varphi$ for $\theta_0 > 0$ and one everywhere smaller than $\varphi$. For the determination of upper and lower approximations, we then have

$$\bar{\theta}_m = \frac{2}{\sqrt{\pi}\,(1+K_\varepsilon)}\left\{\alpha\sqrt{\tau_m} + \sum_{i=1}^m\left[\left(\sqrt{\tau_m - \tau_{i-1}} - \sqrt{\tau_m - \tau_i}\right)\varphi(\tau_i)\right]\right\}, \tag{13}$$

$$\underline{\theta}_m = \frac{2}{\sqrt{\pi}\,(1+K_\varepsilon)}\left\{\alpha\sqrt{\tau_m} + \sum_{i=1}^m\left[\left(\sqrt{\tau_m - \tau_{i-1}} - \sqrt{\tau_m - \tau_i}\right)\varphi(\tau_{i-1})\right]\right\}. \tag{14}$$

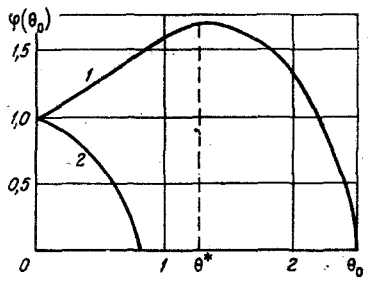


Fig. 1

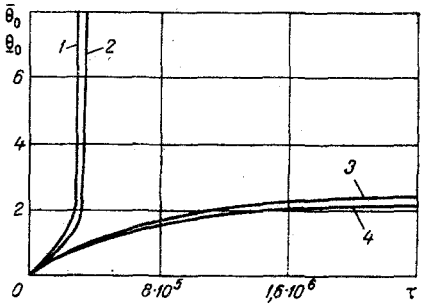


Fig. 2

Fig. 1. Graphs of the dimensionless heat generation function, for $K_\varepsilon = 1000$, $n = 1$, $\alpha = 0$, $\beta = 0.03$, $\theta^* = 1.33$: 1) $a = 0.0004$; 2) $a = 0.0012$.

Fig. 2. Graphs of upper and lower approximations to the dimensionless interface temperature.

Here $\tau_m = m\Delta\tau$ with $\Delta\tau$ denoting the time interval held constant during the computation, $\bar{\theta}_m = \bar{\theta}_0(\tau_m)$ and $\underline{\theta}_m = \underline{\theta}_0(\tau_m)$.

In this way, on each time interval we have a transcendental equation for $\bar{\theta}_m$ and the recurrence formula (14) for $\underline{\theta}_m$.

Relations (13) and (14) are valid only until time $\tau_0$ at which function $\varphi$ has reached its maximum, while later at $\tau > \tau_0$ $\bar{\theta}_m$ is found by (14) and $\underline{\theta}_m$ is found by (13).

The transcendental equation for $\bar{\theta}_m$

$$\bar{\theta}_m = f(\bar{\theta}_m) \tag{15}$$

and $|f'(\bar{\theta}_m)| < k < 1$ was solved by straight iterations, with a known $\bar{\theta}_{m-1}$ taken as the initial approximation. This method fails when $|f'(\bar{\theta}_m)| \geq k$ [8], and the transcendental equation (13) was in this case solved by the elementary method of bisecting the interval. In both cases k was made equal to 0.6.

Ignition is considered to occur at the instant of time which corresponds to the inflection point of curve $\theta_0 = \theta_0(\tau)$. As is well known, at that instant a heterogeneous chemical reaction passes from the kinetic (low-temperature) mode to the diffusion (high-temperature) mode and this determines the condition for ignitability [9]:

$$\left.\frac{d^2\theta_0}{d\tau^2}\right|_{\tau=\tau_*} = 0, \tag{16}$$

where $\tau_*$ denotes the induction or heatup time.

Numerical computations have shown that inflection of the curve depends on the magnitude of parameter $a$. There is an inflection when $a < a_*$ and there is none when $a > a_*$, $a_*$ being some critical value of parameter $a$.

In Fig. 2 are shown $\bar{\theta}_0(\tau)$ and $\underline{\theta}_0(\tau)$ curves for $a < a_*$ and $a > a_*$, with $K_\varepsilon = 1000$, $\alpha = 0$, $\beta = 0.03$, $n = 1$, and $a_* = 0.00032$. Curves 1 and 2 represent, respectively, the upper and the lower approximations to the exact curve $\theta_0(\tau)$ for $a = 0 < a_*$. It is evident here that the distance between the curves increases with time and becomes maximum after the longest time allowed for the computation process. Curves 3 and 4 represent, respectively, the upper and the lower approximations to the exact curve $\theta_0(\tau)$ for $a = 0.0004 > a_*$. There are no inflection points here. At $\tau \to \infty$ both curves approach asymptotically a rather low horizontal line, whereupon the distance between them remains almost constant.

Thus, the absolute error in the determination of $\theta_m$ does not exceed $\bar{\theta}_m - \underline{\theta}_m$ on each step. As to the mathematical convergence of this method, it is determined by the convergence of upper and lower Darbu sums, whose analogs are the sums in (13) and (14), to the exact value of the integral at $\Delta\tau \to 0$.

In Fig. 3 are shown $\bar{\theta}_0(\tau)$ and $\underline{\theta}_0(\tau)$ curves for $a = 0.0004$, with $K_\varepsilon = 1000$, $\alpha = 0$, $\beta = 0.03$, $n = 1$, and $\Delta\tau = 10^4$ or $5 \cdot 10^4$ (curves 1, 1' and 2, 2', respectively). It is evident here that, as $\Delta\tau$ is decreased, both branches come closer, i.e., the absolute error of the method becomes smaller.

After the interval $\Delta\tau$ for a desired accuracy has been established by the method of bilateral approximations, it now becomes worthwhile for machine time economy to use the recurrence formula (14).

We ought to note that such problems can also be solved by the use of a variable $\Delta\tau$ interval which will ensure the required absolute accuracy of the $\theta_0(\tau)$ determination.

3. The method of bilateral approximations can also be used for solving another and more difficult problem concerning heterogeneous ignition, namely where a layer of solid fuel has a finite thickness [9].

The mathematics of the problem reduces to a solution of the following equations in dimensionless form:

$$\frac{\partial\theta_1}{\partial\bar{\tau}} = \frac{\partial^2\theta_1}{\partial\bar{y}^2}, \qquad \bar{y} > 1, \tag{17}$$

$$\frac{\partial\theta_2}{\partial\bar{\tau}} = \mu\frac{\partial^2\theta_2}{\partial\bar{y}^2}, \qquad 0 < \bar{y} < 1, \tag{18}$$

$$\frac{\partial c}{\partial\bar{\tau}} = L\frac{\partial^2 c}{\partial\bar{y}^2}, \qquad \bar{y} > 1 \tag{19}$$

with the initial conditions

$$\theta_1|_{\bar{\tau}=0} = \theta_1|_{\bar{y}=\infty} = \theta_1^0, \qquad \theta_2|_{\bar{\tau}=0} = \theta_2|_{\bar{y}=0} = \theta_2^0, \tag{20}$$

$$\theta_1|_{\bar{y}=1} = \theta_2|_{\bar{y}=1}, \qquad \left(\frac{\partial\theta_1}{\partial\bar{y}} - \omega\frac{\partial\theta_2}{\partial\bar{y}}\right)_{\bar{y}=1} = -\delta\left(\alpha + c_0^n\exp\frac{\theta_0}{1+\beta\theta_0}\right), \tag{21}$$

$$c|_{\bar{\tau}=0} = c|_{\bar{y}=\infty} = 1, \qquad \left.\frac{\partial c}{\partial\bar{y}}\right|_{\bar{y}=1} = \frac{\gamma\delta c_0^n}{L}\exp\frac{\theta_0}{1+\beta\theta_0}. \tag{22}$$

This constraint problem, like the preceding one, reduces to two nonlinear Volterra integral equations for both the temperature and the concentration of the gaseous reagent at the interface:

$$\theta_0 = f_0 + \frac{\delta}{\sqrt{\pi}(1+K_\varepsilon)}\int_0^{\bar{\tau}}\frac{c_0^n\exp\dfrac{\theta_0}{1+\beta\theta_0}}{\sqrt{\bar{\tau}-\bar{t}}}\left[1 + (h-1)\sum_{j=1}^{\infty}h^{j-1}\exp\left(-\frac{j^2}{\mu(\bar{\tau}-\bar{t})}\right)\right]d\bar{t}, \tag{23}$$

$$c_0 = 1 - \frac{a\delta}{\sqrt{\pi}}\int_0^{\bar{\tau}}\frac{c_0^n\exp\dfrac{\theta_0}{1+\beta\theta_0}}{\sqrt{\bar{\tau}-\bar{t}}}\,d\bar{t}, \qquad h = \frac{1-K_\varepsilon}{1+K_\varepsilon}, \tag{24}$$

$$f_0 = \frac{2\alpha\delta}{1+K_\varepsilon}\left\{\sqrt{\frac{\bar{\tau}}{\pi}} + \frac{h-1}{\sqrt{\mu}}\sum_{j=1}^{\infty}\left[\sqrt{\frac{\bar{\tau}\mu}{\pi}}\exp\left(-\frac{j^2}{\mu\bar{\tau}}\right) - j\Phi^*\left(\frac{j}{\sqrt{\mu\bar{\tau}}}\right)\right]h^{j-1}\right\} - \frac{2\theta_1^0}{1+K_\varepsilon}\sum_{j=1}^{\infty}\Phi^*\left(\frac{j}{\sqrt{\mu\bar{\tau}}}\right)h^{j-1}.$$

The proposed replacement of source terms by step functions for the determination of upper and lower approximations yields the following relations:

$$\bar{\theta}_{0m} = \bar{f}_{0m} + \frac{2\delta}{\sqrt{\pi}(1+K_\varepsilon)}\left\{\sum_{k=1}^{m}\varphi(\bar{\theta}_{0k}, \bar{c}_{0k})\left[\sqrt{\bar{\tau}_m - \bar{\tau}_{k-1}} - \sqrt{\bar{\tau}_m - \bar{\tau}_k}\right.\right.$$

$$+ (h-1)\sum_{j=1}^{\infty}\frac{jh^{j-1}}{\sqrt{\mu}}\left[\frac{\exp(-x_{j,k-1})}{\sqrt{x_{j,k-1}}} - \frac{\exp(-x_{j,k})}{\sqrt{x_{j,k}}}\right.$$

$$\left.\left.\left. + \sqrt{\pi}\left(\Phi(\sqrt{x_{j,k-1}}) - \Phi(\sqrt{x_{j,k}})\right)\right]\right]\right\}, \tag{25}$$

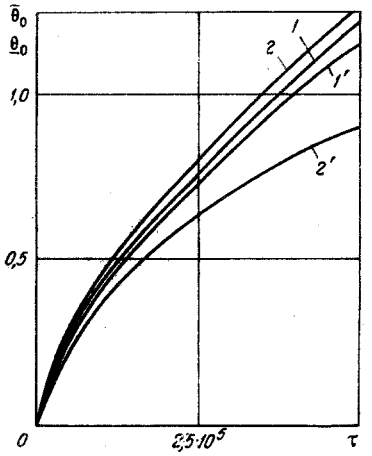


Fig. 3

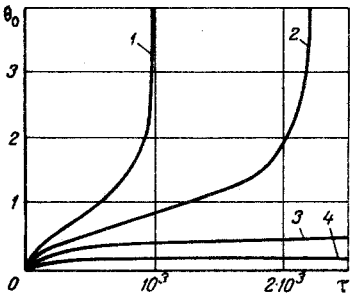


Fig. 4

Fig. 3. Graphs of upper and lower approximations to the function $\theta_0(\tau)$, with different intervals $\Delta\tau$ of numerical integration.

Fig. 4. Graphs of the dimensionless interface temperature $\theta_0(\tau)$, in the ignition mode (1, 2) and in the nonignition mode (3, 4).

$$\underline{\theta}_{0m} = \underline{f}_{0m} + \frac{2\delta}{\sqrt{\pi}\,(1+K_\varepsilon)}\left\{\sum_{k=1}^{m}\varphi\,(\underline{\theta}_{0k},\ \underline{c}_{0k})\left[\sqrt{\bar{\tau}_m-\bar{\tau}_{k-1}}-\sqrt{\bar{\tau}_m-\bar{\tau}_k}\right.\right.$$

$$\left.\left.+\,(h-1)\sum_{j=1}^{\infty}\frac{jh^{j-1}}{\sqrt{\mu}}\left[\frac{\exp(-x_{j,k-1})}{\sqrt{x_{j,k-1}}}-\frac{\exp(-x_{j,k})}{\sqrt{x_{j,k}}}+\sqrt{\pi}\,\left(\Phi(\sqrt{x_{j,k-1}})-\Phi(\sqrt{x_{j,k}})\right)\right]\right]\right\}, \tag{26}$$

$$\bar{c}_{0m} = 1-\frac{2a\delta}{\sqrt{\pi}}\sum_{k=1}^{m}\varphi\,(\underline{\theta}_{0k},\ \underline{c}_{0k})\,(\sqrt{\bar{\tau}_m-\bar{\tau}_{k-1}}-\sqrt{\bar{\tau}_m-\bar{\tau}_k}), \tag{27}$$

$$\underline{c}_{0m} = 1-\frac{2a\delta}{\sqrt{\pi}}\sum_{k=1}^{m}\varphi\,(\bar{\theta}_{0k},\ \bar{c}_{0k})\,(\sqrt{\bar{\tau}_m-\bar{\tau}_{k-1}}-\sqrt{\bar{\tau}_m-\bar{\tau}_k}), \tag{28}$$

$$\varphi(\theta_0,\ c_0) = c_0^n\exp\frac{\theta_0}{1+\beta\theta_0},\quad \theta_{0m}=\theta_0(\tau_m),\quad c_{0m}=c_0(\tau_m),$$

$$x_{j,k-1} = \frac{j^2}{\mu\,(\bar{\tau}_m-\bar{\tau}_{k-1})},\quad x_{j,k} = \frac{j^2}{\mu\,(\bar{\tau}_m-\bar{\tau}_k)}.$$

The sequence of computations: in the first step one computes $\bar{\theta}_{01}$ and $\underline{c}_{01}$, then $\underline{\theta}_{01}$ and $\bar{c}_{01}$, etc. In each step it is necessary to solve a transcendental equation for $\bar{\theta}_{0m}$ and then to apply recurrence formulas to $\underline{\theta}_{0m}$, $\bar{c}_{0m}$, $\underline{c}_{0m}$.

Since for the gaseous and the solid phase $K_\varepsilon \gg 1$ and $h < 1$, hence the expressions for $\bar{f}_{0m}$ and $\underline{f}_{0m}$ contain alternating series. For $\alpha = 0$ we have $f_0 < 0$. In view of this, the series must be cut off after a negative term when an upper approximation is computed and after the following positive term when a lower approximation is computed. The same procedure applies to the computation of sums on the right-hand sides of expressions (25)and (26).

After the optimum $\Delta\tau$ interval has been selected by way of bilateral approximations, the bulk of the computations can be performed with the use of the following recurrence formulas:

$$\theta_{0m} = f_{0m}+\frac{2\delta}{\sqrt{\pi}\,(1+K_\varepsilon)}\left\{\sum_{k=1}^{m}\varphi\,(\theta_{0k-1},\ c_{0k-1})\left[\sqrt{\bar{\tau}_m-\bar{\tau}_{k-1}}\right.\right.$$

$$\left.\left.-\sqrt{\bar{\tau}_m-\bar{\tau}_k}+(h-1)\,\Sigma\right]\right\}, \tag{29}$$

$$c_{0m} = 1-\frac{2a\delta}{\sqrt{\pi}}\sum_{k=1}^{m}\varphi\,(\theta_{0k},\ c_{0k-1})\,(\sqrt{\bar{\tau}_m-\bar{\tau}_{k-1}}-\sqrt{\bar{\tau}_m-\bar{\tau}_k}). \tag{30}$$

The solution of this problem by the described method has made it possible to establish a new limit of heterogeneous ignition $\delta_*$. It appears that the $\theta_0(\tau)$ curves have an inflection when $\delta > \delta_*$ but not when $\delta < \delta_*$. Therefore, a low constant temperature at $y = 0$ impedes and in some cases prevents ignition. This is evident in Fig. 4, where a set of curves is shown for $\delta = 0.2$, 0.4, 0.6, and 0.8 with $K_\varepsilon = 40$, $\alpha = 0$, $\beta = 0.03$, $\mu = 0.001$, $n = 1$, and $\theta_2^0 = 0$. It can be seen here that curves 1 and 2 correspond to ignition while curves 3 and 4 correspond to nonignition.

In determining $\theta_0$, the $\Delta\tau$ interval was selected so as to hold the absolute error within 5%.

It must be noted that the method of bilateral approximations is applicable also to other problems in the theory of heat conduction with nonlinear boundary conditions as, for example, the problem of heat transfer from a gray gas to a solid body, the problem of heat transfer with a moving phase-transformation front, or the problem of heterogeneous combustion.

## NOTATION

$x$ is the space coordinate;

$y = x/r_*$, $\bar{y} = x/r_0$ are the dimensionless coordinates;

$\theta = (T - T_*)E/RT_*^2$ is the dimensionless temperature;

$T$ is the absolute temperature;

$T_*$ is the characteristic temperature: initial interface temperature;

$\tau = t/t_*$, $\bar{\tau} = t/t_0$ are the dimensionless time coordinates;

$t$ is the real-time coordinate;

$t_* = r_*^2 c_1 \rho_1/\lambda_1$, $t_0 = r_0^2 c_1 \rho_1/\lambda_2$ are the time scale factors;

$r_* = (RT^2\lambda_1/C_0^n E q k_0) \cdot \exp(E/RT_*)$ is the length scale;

$r_0$ is the thickness of combustible layer;

$c_i$ is the specific heat of medium i;

$\alpha = (Q/qk_0C_0^n)\exp(E/RT_*)$ is the dimensionless thermal flux;

$Q$ is the thermal flux;

$\rho_i$ is the density of medium i;

$\lambda_i$ is the thermal conductivity of medium i;

$q$ is the thermal effect of reaction;

$k_0$ is the preexponent;

$E$ is the activation energy of heterogeneous reaction;

$R$ is the universal gas constant;

$C_0$ is the initial concentration;

$C$ is the current concentration;

$c = C/C_0$ is the relative concentration at any instant of time;

$K_\varepsilon = \sqrt{\lambda_2\rho_2c_2/\lambda_1\rho_1c_1}$ is the referred coefficient of thermal activity;

$\beta = RT_*/E$ is the dimensionless parameter;

$\mu = \varkappa_2/\varkappa_1$; is the thermal diffusivity of medium i;

$\varkappa_i = \lambda_i/\rho_i c_i$

$n$ is the order of reaction;

$L = D/\varkappa_1$ is the Lewis–Semenov number;

$\gamma = \rho_1 c_1 RT_*^2/qE$ is the dimensionless parameter;

$a = \gamma/\sqrt{L}$;

$\omega = \lambda_2/\lambda_1$;

$\delta = (C_0^n E q k_0 r_0/RT_*^2\lambda_1) \cdot \exp -(E/RT_*)$ is the dimensionless parameter characterizing the thickness of the combustible layer;

$\Phi$ is the error function;

$\Phi^*(x) = 1 - \Phi(x)$.

### Subscripts

$i = 1, 2$;

1 denotes the gaseous phase;

2 denotes the solid phase;

dash above the $\Sigma$ sign indicates an overestimated sum;
dash below the $\Sigma$ sign indicates an underestimated sum.

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