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NUMERICAL SOLUTION OF A TRANSIENT COMBUSTION PROBLEM ON A GRID DYNAMICALLY ADAPTIVE TO THE SOLUTION

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1. Introduction

Basic computational features of nonstationary problems are concerned with such characteristics of solution as formation and propagation of large gradients, surfaces of discontinuities, phase, contact, and free boundaries. Increase of calculation effectiveness with simultaneous improvements of solution quality can be achieved by means of application of adaptive solution-driven grids. One of the most effective approaches to the construction of adaptive grids is the method of dynamic adaptation [1-3]. It is based on the idea of transition to an arbitrary nonstationary coordinate system in which the grid functions and the coordinates of the grid nodes are determined from joint solution of a unified differential model. The transition is carried out automatically by means of the numerical solution of an additional partial differential equation. The right side of the equation contains the transformation function Q which depends on the solution of equations describing physical processes. Successful application of the dynamic adaptation method depends, in many respects, on the form of the transformation function. The optimum transformation is that at which the Q function does not contain free adjusted parameters. In the case of one equation the analysis of the optimum transformation can be done by means of the quasi-stationary method [4]. According to this approach the transformation function is determined from the condition of physical processes being steady-state in the new coordinate system (in computational space). Application of the dynamic adaptation method allows one not only to reduce the number of grid nodes by several orders of magnitude, but also to increase considerably the quality of difference schemes. As demonstrated in [4], applying the dynamic adaptation method it is possible to eliminate the oscillations arising in numerical solution of the Burgers equation in the case of large Reynolds numbers ($Re = 10^6 - 10^7$). Application of the dynamic adaptation method to a nonlinear heat transfer problem (thermal wave propagation) [2,3] allows me to substantially reduce the approximated viscosity of difference schemes.

Determination of the transformation function becomes a very complicated problem in solving a system of equations. The purpose of the present work is to apply the dynamic adaptation method to the solution of a system of nonlinear differential equations of parabolic type. The basic results of modelling are the determination of the normal velocity of flame propagation and diffusive-thermal structure of the flame front in different regimes. The basic feature of the problem investigated is the oscillatory character of a solution.

2. Problem statement

The model problem of the propagation of the laminar flame front is considered under the assumption that the combustion process is isobaric and heat transfer in matter proceeds by diffusion mechanism. In the approximation considered the rate of an exothermal reaction depends linearly on the matter density ρ and exponentially on the temperature T. The basis of laminar flame propagation in a fixed gas mixture is the mechanism of heattransfer from the area of burnout high-temperature gas to more cold layers of the nonreacting mixture. Under the assumptions made the combustion problem is described by a system of two nonlinear equations of parabolic type, namely, heat-transfer and diffusion equations with constant coefficients of thermal diffusivity a and diffusion D. If the values of these coefficients are equal (the Lewis number $Le = 1$), then the combustion front propagates with a constant velocity.

When $Le < 1$ and at certain additional relations, the combustion process becomes pulsing. The high rate of chemical transformation of a reactant and slow propagation of thermal perturbations in the nonreacting mixture lead to the formation of a narrow combustion zone characterized by the large temperature and density gradients.

Following [3], consider a one-dimensional rod in the physical space $\Omega_{\tilde{x},\tilde{t}}$ consisting fully of the substance A. The rod is heated on the left end and burns out completely with an increase in the substance temperature.

In the physical space $\Omega_{\tilde{x},\tilde{t}}$ in a dimensional form the model problem is described by the following equations:

$$\frac{\partial \tilde{\rho}_A}{\partial \tilde{t}} = D_A \frac{\partial^2 \tilde{\rho}_A}{\partial \tilde{x}^2} - \tilde{\rho}_A K_A \exp\left(-\frac{E_A}{R\tilde{T}}\right), \tag{1}$$

$$C_p \rho_0 \frac{\partial \tilde{T}}{\partial \tilde{t}} = k \frac{\partial^2 \tilde{T}}{\partial \tilde{x}^2} + \Delta h_A \tilde{\rho}_A K_A \exp\left(-\frac{E_A}{R\tilde{T}}\right), \tag{2}$$

$$0 = \tilde{x}_0 \le \tilde{x} \le \tilde{x}_1 = L, \quad \tilde{t} \ge 0,$$

where $\tilde{\rho}_A$ is the substance density, $\tilde{T}$ is the temperature; $\tilde{t}$ and $\tilde{x}$ are the independent variables of time and spatial coordinate; Δh_A is the specific heat of combustion; D, k, C_p and ρ_0 are the diffusion, thermal conduction, specific heat coefficients , and initial substance density, respectively; E_A is the activation energy of reaction. Denote $\alpha = \dfrac{k}{C_p \rho_0}$, $Le_A = \dfrac{D_A}{\alpha}$ and introduce the following dimensionless variables:

$$\rho_A = \frac{\tilde{\rho}_A}{\rho_0}, \quad x = \frac{\tilde{x}}{L}, \quad t = \frac{\tilde{t}\alpha}{L^2}, \quad T = \frac{\tilde{T} C_p}{\Delta h_A}, \quad \theta_A = \frac{E_A C_p}{R(\Delta h_A)}, \quad A_A = \frac{K_A L^2}{\alpha}.$$

In the dimensionless variables the Eqs. (1) and (2) take the form:

$$\frac{\partial \rho_A}{\partial t} = Le_A \frac{\partial^2 \rho_A}{\partial x^2} - \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right), \tag{3}$$

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right), \tag{4}$$

where $x_0 \le x \le x_1$, $t \ge 0$, $x, t \in \Omega_{x,t}$.

The initial and boundary conditions are:

$$t = 0: \quad T(x,0) = T_0; \quad \rho_A(x,0) = \rho_0,$$

$$x = x_0: \quad T(x,t) = \begin{cases} T_0 + c^* t, & t \le \dfrac{1}{c} \\ T_F, & t \ge \dfrac{1}{c} \end{cases}, \quad \left.\frac{\partial \rho_A}{\partial x}\right|_{x_0} = 0. \tag{5}$$

$$x = x_L: \quad \left.\frac{\partial T}{\partial x}\right|_{x_L} = 0, \quad \left.\frac{\partial \rho_A}{\partial x}\right|_{x_L} = 0.$$

3. Problem formulation in an arbitrary nonstationary coordinate system

Introduce the computational space $\Omega_{q,\tau}$: $0 = q_0 \le q \le q_L$, $\tau > 0$. Transition from the physical space $\Omega_{x,t}$ into the computational one is carried out by means of general coordinate transformation $x = \xi(q,\tau)$, $t = \tau$, which has inverse transformation $q = \varphi(x,t)$, $\tau = t$. The Jacobian of the transformation is $\psi = \dfrac{\partial x}{\partial q}$. The partial derivatives of the dependent variables are expressed in an ordinary way:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial q}{\partial t}\frac{\partial}{\partial q} = \frac{\partial}{\partial \tau} - \frac{\partial x}{\partial \tau}\frac{1}{\psi}\frac{\partial}{\partial q} = \frac{\partial}{\partial \tau} + \frac{Q}{\psi}\frac{\partial}{\partial q}, \quad \frac{\partial}{\partial x} = \frac{\partial q}{\partial x}\frac{\partial}{\partial q} = \frac{1}{\psi}\frac{\partial}{\partial q},$$

where $\dfrac{\partial x}{\partial \tau} = -Q$ denotes the velocity of the nonstationary coordinate system.

In the new variables q, τ problem (3), (4) is written as:

$$\frac{\partial T}{\partial \tau} + \frac{Q}{\psi}\frac{\partial T}{\partial q} = -\frac{1}{\psi}\frac{\partial W}{\partial q} + \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right), \quad \text{where } W = -\frac{1}{\psi}\frac{\partial T}{\partial q},$$

$$\frac{\partial \rho_A}{\partial \tau} + \frac{Q}{\psi}\frac{\partial \rho_A}{\partial q} = Le_A \frac{1}{\psi}\frac{\partial}{\partial q}\frac{1}{\psi}\frac{\partial \rho_A}{\partial q} - \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right), \tag{6}$$

$$\frac{\partial \psi}{\partial \tau} = -\frac{\partial Q}{\partial q}, \quad \frac{\partial x}{\partial q} = \psi.$$

In the $\Omega_{q,\tau}$ space the initial and boundary conditions have the form:

$$T(q_0, t) = \begin{cases} T_0 + c^* t, & t \le \dfrac{1}{c} \\ T_F, & t \ge \dfrac{1}{c} \end{cases}, \quad \left.\frac{\partial T}{\partial q}\right|_{q_L} = 0, \quad \left.\frac{\partial \rho_A}{\partial q}\right|_{q_0} = 0, \quad \left.\frac{\partial \rho_A}{\partial q}\right|_{q_L} = 0. \tag{7}$$

Prior to the finite-difference approximation of differential model (6) it is expedient to present it in a fully divergent form:

$$\frac{\partial(\psi T)}{\partial \tau} = -\frac{\partial W}{\partial q} - \frac{\partial(QT)}{\partial q} + \psi \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right), \tag{8}$$

$$\frac{\partial(\psi \rho_A)}{\partial \tau} = -Le_A \frac{\partial C_A}{\partial q} - \frac{\partial(Q\rho_A)}{\partial q} - \psi \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right), \tag{9}$$

$$\frac{\partial \psi}{\partial \tau} = -\frac{\partial Q}{\partial q}, \quad \frac{\partial x}{\partial q} = \psi, \qquad C_A = -\frac{1}{\psi}\frac{\partial \rho}{\partial q}. \tag{10}$$

To increase substantially the effectiveness of the dynamic adaptation method we present the (8)—(10) as a free boundary problem. Taking into account that the combustion process is initiated on the left boundary $q = q_0$, and then propagates through the cold background toward the right boundary $q = q_L$, it is efficient to exclude from consideration the area which is not reached as yet by the combustion wave. It is not difficult to perform this procedure in the arbitrary non-stationary coordinate system. For this purpose, we define the arbitrary point $q_* \in (q_0, q_L)$: $q_* > q_0$ and $q_* \ll q_l$ to be a new boundary with the following boundary conditions [2]:

$$T(q_*, t) = T_0, \quad u = \lim_{q \to q_*} \frac{k}{cT}\frac{1}{\psi}\frac{\partial T}{\partial q}. \tag{11}$$

Until the perturbation reaches the point $q = q_*$ the boundary remains fixed. Its movement begins with the arrival of the thermal wave and finishes as soon as the point $q = q_L$ is reached.
Finally, the boundary and initial conditions for the Eq. 10 are written:

$$Q(q_0, t) = 0, \quad Q(q_*, t) = -u, \quad \psi(q, 0) = 1. \tag{12}$$

4. Choice of the transformation function Q

Definition of the function Q determines a specific form of coordinate transformation. The function also presents a characteristic to control the movement of the grid nodes. Therefore, a correct choice of the transformation function in the dynamic adaptation method is of great importance and should provide the movement of the grid nodes to be consistent with the behavior of the sought-for solution.

Let us define Q from the following considerations. For the complete consistency of the adaptation mechanism with the unknown solution the function should depend on the solution of the set of equations (6). Also, it should not contain free parameters. For definition of the necessary transformation function we take advantage of the quasi-stationary method [4] and choose a nonstationary coordinate system, providing the time-dependent derivatives of the solution being equal to zero or being small enough.
Assume that the above coordinate system is found and $\partial(T + \rho_A)/\partial\tau = 0$ condition is fulfilled. Then the set of equations (6) takes the form:

$$\frac{Q}{\psi}\frac{\partial T}{\partial q} = \frac{1}{\psi}\frac{\partial}{\partial q}\frac{1}{\psi}\frac{\partial T}{\partial q} + \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right),$$

$$\frac{Q}{\psi}\frac{\partial \rho_A}{\partial q} = Le_A \frac{1}{\psi}\frac{\partial}{\partial q}\frac{1}{\psi}\frac{\partial \rho_A}{\partial q} - \rho_A A_A \exp\left(-\frac{\theta_A}{T}\right). \tag{13}$$

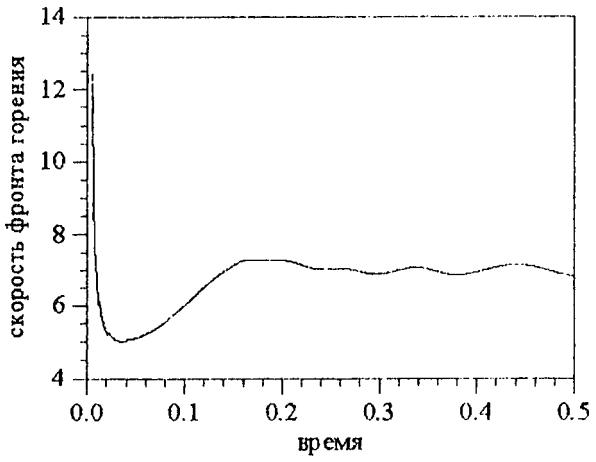

Fig. 1. The flame front propagation velocity, computed on the adaptive grid with $N = 30$ at $Le = 0.6$, $A = 10^9$, $\theta_A = 17$.

Resolving (13) with respect to Q we obtain:

$$Q = \frac{\frac{1}{\psi}\left(Le_A \frac{\partial}{\partial q}\left|\frac{\partial \rho_A}{\partial q}\right| + \frac{\partial}{\partial q}\left|\frac{\partial T}{\partial q}\right|\right)}{\left|\frac{\partial}{\partial q}(\rho_A + T)\right| + \frac{Reg}{h}} + \frac{\left(\frac{\partial}{\partial q}\frac{1}{\psi}\right) * \left(Le_A\left|\frac{\partial \rho_A}{\partial q}\right| + \left|\frac{\partial T}{\partial q}\right|\right)}{\left|\frac{\partial}{\partial q}(\rho_A + T)\right| + \frac{Reg}{h}} + \psi \frac{\rho_A A_A \exp\left(-\frac{\theta_A}{T}\right)}{\left|\frac{\partial}{\partial q}(\rho_A + T)\right| + \frac{Reg}{h}}. \qquad (14)$$

The first and third terms in this formula ensure concentration of the grid nodes, and the second term limits the minimum distance between two neighboring nodes. The additional term Reg/h is introduced to prevent the denominator from being equal to zero. The first derivatives of density and temperatures are taken by absolute values to account for nonmonotonous behavior of the solution.

5. Finite-difference approximation

For solution of problems (3)—(5) in the variables (x, t) and (8)—(12) in the variables (q, τ) we introduce two discrete spaces $\omega_{h_x}^{\Delta t}$ and $\omega_{h_q}^{\Delta \tau}$:

$$\omega_{h_x}^{\Delta t} = \left\{(x_i, t^j); x_{i+1} = x_i + h_x, t^{j+1} = t^j + \Delta t^j; i = 0, 1, \ldots, N, j = 0, 1, \ldots, J\right\},$$

$$\omega_{h_q}^{\Delta \tau} = \left\{(q_i, \tau^j); q_{i+1} = q_i + h_q, q_{i+1/2} = q_i + h_q/2, \tau^{j+1} = \tau^j + \Delta \tau^j; i = 0, 1, \ldots, N, j = 0, 1, \ldots, J\right\}.$$

The differential equations (3), (4) are approximated by the set of finite-difference schemes:

$$\begin{aligned} \frac{\rho_{Ai}^{j+1} - \rho_{Ai}^{j}}{\Delta t^j} &= Le_A \frac{\rho_{Ai-1}^{(\sigma_1)} - 2\rho_{Ai}^{(\sigma_1)} + \rho_{Ai+1}^{(\sigma_1)}}{h_x^2} - \rho_{Ai}^{(\sigma_1)} A_A \exp\left(-\frac{\theta_A}{T_i^{(\sigma_2)}}\right), \\ \frac{T_i^{j+1} - T_i^{j}}{\Delta t^j} &= Le_A \frac{T_{Ai-1}^{(\sigma_2)} - 2T_i^{(\sigma_2)} + T_{i+1}^{(\sigma_2)}}{h_x^2} + \rho_{Ai}^{(\sigma_1)} A_A \exp\left(-\frac{\theta_A}{T_i^{(\sigma_2)}}\right). \end{aligned} \qquad (15)$$

Here $f_i^{*(\sigma)} = \dfrac{f_{i+1/2}^{(\sigma)} + f_{i-1/2}^{(\sigma)}}{2}$.

6. Results of modelling

The effectiveness of the algorithms used is determined by comparison of the computer run time with the number of grid nodes needed to compute the same variants on adaptive and fixed Eulerian grids. The comparison has shown that converging values of the velocity u in all the regimes can be achieved at N=30 on adaptive grids and N ranging from 1000 to 3000 (depending on a specific regimes) is required on fixed grids. The consumption of computer run time is 5-20 times less for the adapted grids than for the Eulerian ones. Moreover, the calculations have shown that the difference schemes on the adapted grids have considerably

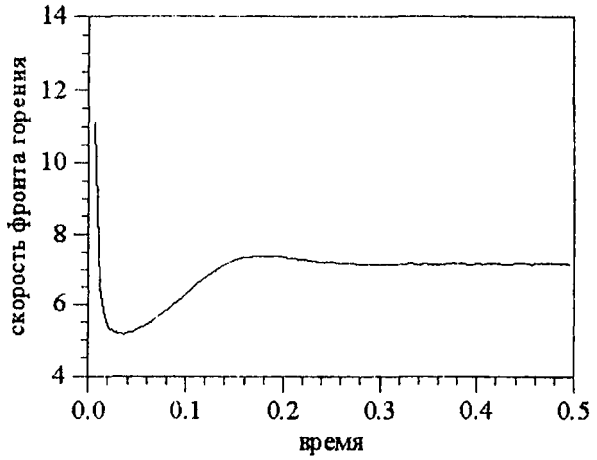

Fig. 2. The flame front propagation velocity, computed on the fixed grid with $N = 3000$ at $Le = 0.6$, $A = 10^9$, $\theta_A = 17$.

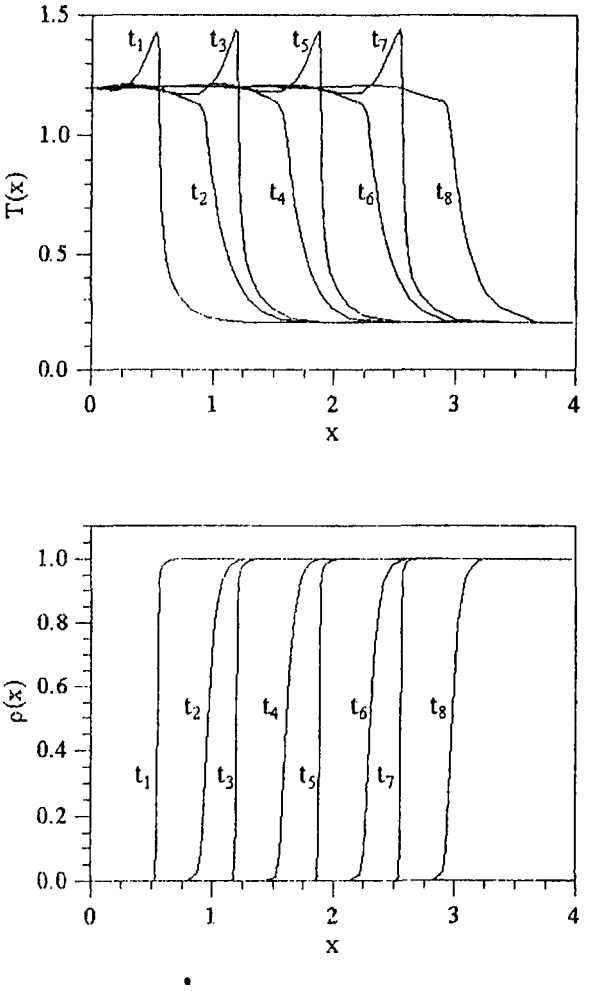

Fig. 3. Temperature T and density ρ plots versus spatial coordinate at the time moments $t_1 - t_8$ at $Le = 0.3$, $A = 10^{10}$, $\theta_A = 18$.

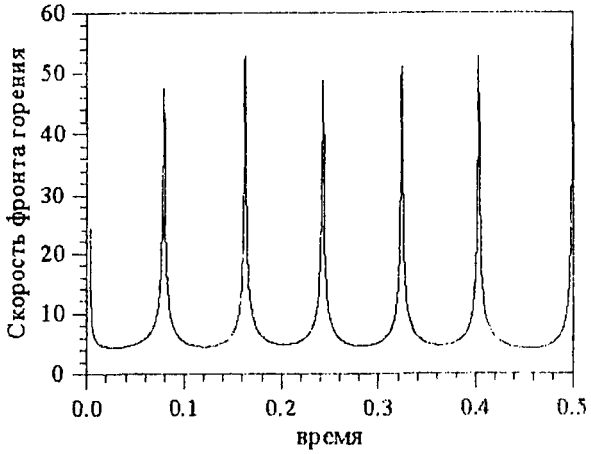

Fig. 4. Combustion front velocity at $Le = 0.3$, $A = 10^{10}$, $\theta_A = 18$.

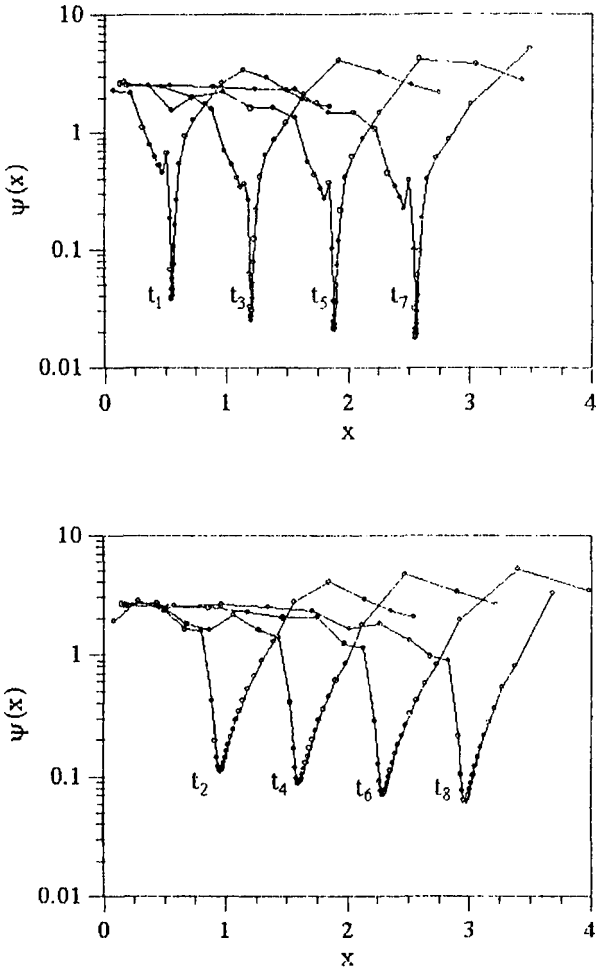

Fig. 5. Dimensionless space steps at the time moments of flases (a) and dipressions (b) at $Le = 0.3$, $A = 10^{10}$, $\theta_A = 18$.

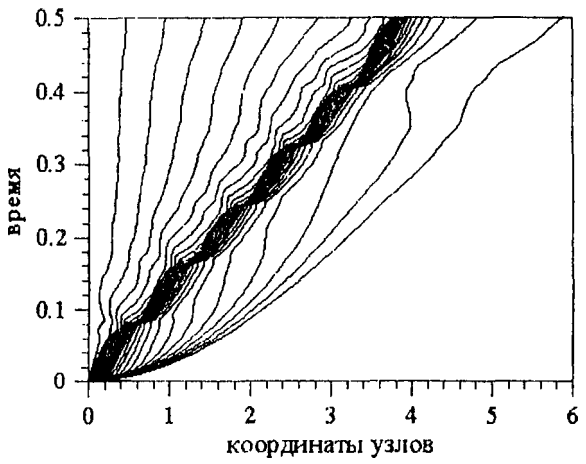

Fig. 6. Nodes movement digramm at $Le = 0.3$, $A = 10^{10}$, $\theta_A = 18$.

smaller schematic viscosity. It is proved by the fact, that in adaptive grid computations at $A_A = 10^9$ and $\theta_A = 17$ an oscillatory mode of solution is observed already at $Le = 0,6$, Fig. 1, while complete lack of oscillations is observed on an Eulerian grid with $N = 3000$ and oscillations appears only at a smaller Lewis number $Le = 0,5$.

The mathematical modelling of different combustion regimes allows one to establish:

1. When $Le \to 1$, steady combustion regimes are realized with a constant velocity of flame front propagation. The isentropic combustion temperature, $T = T_a$, is established behind the front.

2. When $Le > 1$, a constant propagation velocity is also established, but there is an excess of enthalpy and temperature $T > T_a$.

3. At small values of $Le \ll 1$ nonstationary combustion is observed with periodic oscillations of temperature, concentration, and reaction rate, Figs. 3,4. The periodic concentrations of grid nodes on the motion diagram, Figs. 5,6, correspond to these oscillations. The dynamics of the adapted grid nodes is also characterized by spatial profiles of the function ψ shown in Figs. 5,6 for the different time moments. The function $\psi(x)$ characterizes variation of the spatial step h_x and shows, how many times the distance changed between subsequent grid nodes in the physical space. At the moments of flashes corresponding to maximum values of temperature and velocity the nodes are concentrated in the vicinity of the thermal and diffusion fronts. These moments correspond to sharp falls on the $\psi(x)$ plots.

7. Conclusion

The approach is presented to define the transformation function for a set of parabolic type equations and is illustrated by solution of an unsteady combustion problem. The construction of a transformation function without free adjusted parameters makes the method of dynamic adaptation an effective tool for research of the oscillatory solutions, typical for unstable regimes.

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