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RESEARCH ARTICLE

Simulation of the detonation regime excited by combustion process turbulence

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Abstract

Objectives. The work considers critical processes involving excess energy, which include combustion and explosion, destruction of materials, crystallization, sintering of materials, etc. The results of numerical modeling of the turbulence of the combustion process (laminar–turbulent transition) and the patterns of phenomena associated with the laminar–turbulent transition in critical processes are studied.

Methods. Thermodynamic analysis was used to outline the trajectories of a system's evolution and identify areas of laminar combustion stability during combustion, as well as metastable and labile regions where laminar combustion is unstable. An energy analysis approach was used to solve research problems involving the study of the redistribution of excess energy and the formation of distinctive structural features and parameters of the object and processes.

Results. The results of a numerical experiment of the vibrational turbulence regime of the combustion process are presented as an interaction of the Rauschenbach resonance and laminar–turbulent transition. The resonance occurring during kinetic energy pumping, which implements the discharge of excess energy, is modeled on a variety of local equilibrium. In order to explain the new concepts that arise in this case, the resonance of the adiabatic hydrodynamic process is described. The possibility of avoiding resonance through the mechanism of dumping excess energy by turbulence of the laminar process is confirmed by the results of field experiments.

Conclusions. The possibility of avoiding resonance in vibrational combustion due to disruption of the local equilibrium from the manifold by turbulence of the laminar process (approximation of local equilibrium) during pumping kinetic energy is demonstrated. During the combustion process, areas of laminar combustion stability are identified, along with metastable and labile areas where laminar combustion is unstable. However, this does not mean that signs of turbulence will not be observed in the stability region in its developed state: in these regions the diffusion of perturbations will blur them, whereas in the instability regions the process of negative (Cahn) diffusion will result in their concentration. It can be assumed that the instability regions of a homogeneous system are sources of perturbations, while the stability regions are sinks.

Keywords: laminar-turbulent transition, detonation, combustion, energy, diffusion

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НАУЧНАЯ СТАТЬЯ

Моделирование детонационного режима, возбуждаемого турбулизацией процесса горения

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Резюме

Цели. Объектом исследования являются критические процессы с избыточной энергией, к которым относятся процессы горения и взрыва, разрушения материалов, кристаллизации, спекания материалов и др. Предметом исследования являются результаты численного моделирования турбулизации процесса горения (ламинарно-турбулентного перехода) и закономерностей явлений, связанных с ламинарно-турбулентным переходом в критических процессах.

Методы. Использован термодинамический анализ, обозначивший траектории эволюции системы и показавший, что в процессе горения существуют области устойчивости ламинарного горения, а также метастабильные и лабильные области, где ламинарное горение неустойчиво. Применен энергетический подход к решению задач исследования, при котором основное внимание уделяется вопросам изучения перераспределения избыточной энергии и формирования отличительных признаков структуры и параметров объекта и процессов.

Результаты. Представлены результаты численного эксперимента вибрационного режима турбулизации процесса горения, как взаимодействие резонанса Раушенбаха и ламинарно-турбулентного перехода. На многообразии локального равновесия смоделирован резонанс при накачке кинетической энергии, реализующий сброс избыточной энергии. Для пояснения возникающих при этом новых понятий описан резонанс адиабатического гидродинамического процесса и показана возможность избежать резонанс через механизм сброса избыточной энергии турбулизацией ламинарного процесса, что подтверждается результатами натурных экспериментов.

Выводы. Показано, что в вибрационном горении можно избежать резонанс за счет срыва с многообразия локального равновесия турбулизацией ламинарного процесса (приближения локального равновесия) при накачке кинетической энергии. В процессе горения существуют области устойчивости ламинарного горения, а также метастабильные и лабильные области, где ламинарное горение неустойчиво. Это не означает, что в области устойчивости не будут наблюдаться признаки турбулентности при ее развитом состоянии и в этих областях диффузия возмущений будет их размывать, тогда как в областях неустойчивости процесс «отрицательной» (кановской) диффузии будет их концентрировать. Сделано предположение, что области неустойчивости гомогенной системы являются источниками возмущений, а области устойчивости – «стоками».

Ключевые слова: ламинарно-турбулентный переход, детонация, горение, энергия, диффузия

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INTRODUCTION

According to the logic of the Cahn–Hilliard formulations of the theory of nonequilibrium phase transitions [1, 2] and Debye's theory of critical opalescence [3], critical phenomena are described solely as excess energy processes while omitting the details of chemistry. The degradation of a laminar process by a turbulent process is shown to lead to energy dissipation [4–8]. Turbulence is hypothesized to be "one of the mechanisms of nucleation of a stable detonation zone" [4]. This hypothesis is confirmed experimentally by Shiplyuk[1] et al. [9–11] by applying an adjustable inhomogeneity on a streamlined surface. Of particular interest here is the location and timing of the disruption of the local equilibrium manifold during the release of excess energy by turbulence of the process.

In the present work, energy is conceptualized in different forms:

(a) chemical energy is represented in terms of concentrations;
(b) the nonequilibrium part of the free energy according to Cahn is the concentration gradient;
(c) the mechanical component is in the form of a "gradient" of stresses (structured as a spring), which produces a coherent spinodal [11];
(d) by analogy, the kinetic energy of vortices (as quasi-particles, fluid particles of continuum mechanics) can be added.

The energy method is characterized by its clarity and simplicity for solving a wide range of problems. However, in order to outline the simplest practical methods of acting on an oscillating system and to provide its full theoretical description, it is necessary to take feedback mechanisms into account. A well-known but poorly studied transient process involves switching from laminar to turbulent modes.

PROBLEM STATEMENT FOR THE SIMULATION OF TURBULENCE IN VIBRATING COMBUSTION

The present work sets out to solve the following problems:

- derivation of the model of laminar combustion in the field of gravity with energetic consideration of hydrodynamics;
- vortex energy, degradation measure of laminar combustion, entropy, and free energy of the turbulence process of laminar combustion;
- sign-variable diffusion, an analog of the Cahn–Hilliard operator in the internal energy equation (closure of the disturbance from the manifold of the laminar combustion process);
- numerical experiment of the vibrational mode of combustion turbulence as an interaction of Rauschenbach resonance [5] and laminar–turbulent transition.

TURBULENCE MECHANISM FOR VIBRATIONAL COMBUSTION

In [6–8], a vibrational explosion (resonance when pumping kinetic energy) implementing excess energy discharge is modeled on the local equilibrium manifold (within the laminar process of the local equilibrium approximation). In [8], the resonance of an adiabatic hydrodynamic process is described to explain the new concepts arising in this case. The possibility of avoiding the resonance through the mechanism of excess energy discharge by turbulence of the laminar process is empirically confirmed in [12].

[1] Shiplyuk A.N. *Growth of perturbations and control of boundary layers at hypersonic speeds*. Dr. Sci. Thesis (Phys.-Math.). Novosibirsk, 2005. 320 p. (in Russ.).

According to I.G. Barenblatt, a transformed state occurs in vibrational combustion where the mechanism of excess energy release is either resonance or turbulence of the process. For a single active component, the global inhomogeneity of the system can be characterized as an inhomogeneous enthalpy distribution across the flow (mixture). When pumping kinetic energy in the combustion process in the phase-space field of gravity described by variables (volume V, pressure P, temperature T, reduced amount of active component n, entropy S, internal energy E, velocity of the active component u_1, and velocity of the passive component u_2), the enthalpy increment is a full differential on the local equilibrium manifold [5], on which the laminar process (in the local equilibrium approximation) is described by equations (1)–(4) of the classical two-component model of the combustion process in the gravitational field:

$$\partial_t \rho + \partial_x(\rho U) = \varepsilon_R \Delta\rho, \tag{1}$$

$$\partial_t((1-c_0 n)\rho u_2) + \partial_x((1-c_0 n)\rho u_2^2) + \partial_x P = \\ = \varepsilon_R \Delta u_2 + \varepsilon_g (1-c_0 n),$$

$$\partial_t(c_0 n \rho u_1) + \partial_x(c_0 n \rho u_1^2) + \partial_x P = \\ = \varepsilon_R \Delta u_1 + \varepsilon_g c_0 n \rho,$$

$$\rho \frac{d}{dt} E + P \mathrm{div} U = \varepsilon_R \Delta E,$$

where ρ is density; x is the spatial variable; t is time; c_0 is the concentration of active component; ε_g is the free fall acceleration; ε_R = 1/Re; Re is the Reynolds number; $\varepsilon_R = \varepsilon / (\rho_* U_* L_*)$; ρ_* is the characteristic density of homogeneous mixture; U_* is the characteristic velocity of homogeneous mixture; L_* is the characteristic size of medium; ε is the kinetic viscosity; the average velocity of mixture is $U = c_0 n u_1 + (1-c_0 n)u_2$; $\frac{d}{dt} = \partial_t + U\partial_x$; kinetic equations [13, 14] are:

$$\rho c \frac{d}{dt} T = \partial_x(\lambda \partial_x T) + QW(n,T), \tag{2}$$

where c is the molar concentration and Q is heat.

$$\rho \frac{d}{dt} n = \partial_x(\rho D \partial_x NNn) - W(n,T),$$

where D is the mobility coefficient; NNn is the reduced amount of the active component of the two-component mixture.

$$W = k_0 \rho n^\beta \mathrm{e}^{-\frac{E_*}{RT}}, \tag{3}$$

where k_0 is the reaction rate constant at temperature; β is the reaction order; R is the universal gas constant; E_* is activation energy.

The closing equations in this case are the equations of state:

$$P = (\gamma - 1)\rho E + \frac{P_{\mathrm{ad}}^0}{\rho_0}\rho - \rho g(x, e_1) + \\ + TS\rho + n\rho\mu + RnT\rho, \tag{4}$$

where γ is the adiabatic exponent; P_{ad}^0 is the initial adiabatic pressure; ρ_0 is the density; g is the gravitational constant; e_1 = 1, 0, 0; μ is the chemical potential.

$$S + nS + n\left(\frac{d\mu_0(T)}{dT} + R\ln\left(\frac{nT\rho^2}{n_0 T_0 \rho_0^2}\right)\right) = 0, \tag{5}$$

where μ_0 is the chemical potential at the input T_0 is the temperature; n_0 is the reduced amount of active component.

Here, the primary hypothesis states that the mechanism of the laminar–turbulent transition in the combustion process during the kinetic energy pumping is represented by diffusive stratification. In the one-dimensional case, this is implemented by a striped structure of interleaved layers with large (turbulent layers) and small (laminar layers) gradients of variables. The increased entropy of the system during the transition from the laminar to the turbulent state is represented in the form of the entropy of mixing of specific volumes (layers of an ideal mixture) having different values of the hydrodynamic component of the enthalpy, as well as the work against gravity, the energy component of the combustion process, and the component due to compressibility.

TURBULENCE OF VIBRATIONAL COMBUSTION. PUMPING

For vibrational combustion, it is natural to take the ratio of the vortex energy density H_{M} to the kinetic energy density (a measure of laminar combustion degradation) as a measure of the process degradation due to the laminar–turbulent transition, as follows:

$$h = \frac{\rho H_{\mathrm{M}}}{\frac{1}{2}\rho U^2},$$

where M is the local equilibrium manifold.

At the same time, the energetic influence of gravity on the laminar–turbulent transition in the combustion process is taken into account. To construct the second order phase transition, it is first necessary to construct an analog of the Landau–Ginzburg potential (specific Gibbs free energy). We investigate the possibility of extending the concept of nonequilibrium phase transitions as conceptualized in the Cahn–Hilliard spinodal decomposition theory to include the laminar–turbulent transition of the kinetic energy pumping combustion process. Here, the condition for breaking the local equilibrium manifold is formulated using the degradation measure of the laminar combustion process. We now turn to new variables. We introduce pumping by analogy with the laser terminology of Haken [15]:

$$\xi = \frac{(\gamma-1)\rho E}{\rho \tilde{U}^2}, \tag{6}$$

where $\tilde{U}$ is the internal energy.

We denote the laminar–turbulent transition variable by

$$h = \frac{H_M}{\rho U^2} = \xi + \nu,$$

where the number of vibrational turbulence is:

$$\nu = \frac{-\rho_0 E_0 - \rho^3 g(x,e_1) + \frac{P_{ad}^0}{\rho_0}(\rho-\rho_0) + \left[-T\frac{d\mu_0(T)}{dT} + \mu_0(T) - RT\right]n\rho}{\rho \tilde{U}^2},$$

where E_0 is the initial internal energy.

The vortex energy is as follows:

$$H_M = (\gamma-1)(\rho E - \rho_0 E_0) - \rho g(x,e_1) + \frac{P_{ad}^0}{\rho_0}(\rho-\rho_0) + \left[-T\frac{d\mu_0(T)}{dT} + \mu_0(T) - RT\right]n\rho =$$
$$= P_{ad,g} - P_{comb} + \left[-T\frac{d\mu_0(T)}{dT} + \mu_0(T)\right]n\rho - (\gamma-1)\rho_0 E_0 - P_{ad}^0,$$

where $P_{ad,g} = (\gamma-1)\rho E + \frac{P_{ad}^0}{\rho_0}\rho - \rho^3 \varepsilon_g(x,e_1)$ is the pressure of adiabatic hydrodynamic process in the gravity field and $P_{comb} = RTn\rho$ is the Mendeleev–Clapeyron equation.

The initial partial pressure $P_{ad}^0 = \text{const}$, as well as $\rho_0 = \text{const}$, and the initial internal energy $E_0 = \text{const}$.

As shown below, the condition for the excitation of turbulence has the form of $\nu \ll 1$. It should be noted that, for $\nu \to 0$, a larger U^2 denotes more developed turbulence (ν is an analog of the Reynolds number).

The condition for the nucleation of the laminar–turbulent transition in vibrational combustion (feedback) is that the vibrational turbulence number is sufficiently small ($\nu \to 0$) provided that $U^2 \to \infty$. The latter is true if

$$\frac{Tn}{U^2} \to 0, \tag{7}$$

being verified by a numerical experiment.

LAMINAR–TURBULENT TRANSITION POTENTIAL OF THE COMBUSTION PROCESS, $\tilde{F}(\xi, \nu)$

The laminar–turbulent transition in vibrational combustion occurs when the velocity of the passive component at the input increases. This corresponds to phase transitions in systems of poorly soluble liquids with a lower critical point for stratification (in such systems, stratification occurs when the temperature increases, which corresponds to an increase in enthalpy; in hydrodynamic systems, it corresponds to an increase in the hydrodynamic component of the total enthalpy). It is known from experiments that a mixture of turbulent and laminar layers (sponges in Landau's terminology) can be considered as a perfect mixture for which the entropy of the laminar–turbulent transition process is:

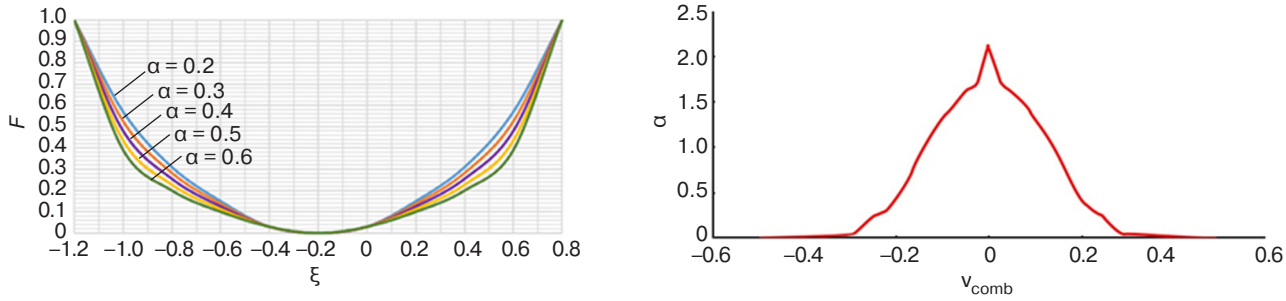
$$s = (h) = -(h^2\ln(h^2) + (1-h^2)\ln(1-h^2)), \tag{8}$$

$$h = \xi + \nu,\ \nu \to 0, \text{ if } |U| \to \infty. \tag{9}$$

The distribution h represents the excess enthalpy of an inhomogeneous thermodynamic system with respect to a homogeneous one. Here, h^2 and s are the dimensionless enthalpy and entropy of the laminar–turbulent transition, respectively. The dimensionless Gibbs free energy G of the laminar–turbulent transition process is given by

$$F(\xi;\alpha,\nu_{comb}) = h_{comb}^2 - \alpha(\nu_{comb})h_{comb}^2 s(h_{comb}^2), \tag{10}$$

which is an analog of the Gibbs–Helmholtz equation $\Delta G = \Delta H - T\Delta S$, where the intensive variable T (temperature) is represented by the parameter $\alpha(\nu_{comb})h_{comb}^2$, reflecting the relationship between temperature and enthalpy H due to the energy intensity of the medium (analog of the heat capacity); α is a parameter on the design interval; ν_{comb} is the number



(a) (b)

Fig. 1. (a) Potential $F(\xi; \alpha; v_{comb})$ at $v = 0.2$ and different values of $\alpha = 0.2, 0.3, 0.4, 0.5, 0.6$; (b) dependence $\alpha(v_{comb})$

of turbulence at heat pumping; h_{comb} is the calculated enthalpy. Here, the function $\alpha(v_{comb})$ is defined by the graph shown in Fig. 1b. The plots of the potential $F(\xi;\alpha,v_{comb})$ at $v = 0.2$ and different values of α are shown in Fig. 1a.

We perform the correction of the potential $F(\xi;\alpha,v_{comb})$ according to [13], as follows:

1) for $-1 < v_{comb} \le 0$, $-1 + |v| < \xi < 1 + |v|$ we set:

$$\tilde{F}(\xi,v_{comb}) = \begin{cases} F(\xi,v_{comb}), & 0 \le \xi < 1+|v_{comb}|, \\ \gamma_-(h^2(\xi) - h^2(0) + F(0,v_{comb})), & \xi < 0. \end{cases} \quad (11)$$

The constant γ_- is found from the condition

$$2\gamma_- v = \frac{d}{d\xi}F(0,v) = 2v(1 + 2\alpha v^2 \ln(v^2) + \alpha(1 - 2\alpha v^2)\ln(1 - v^2))$$

or

$$\gamma_- = (1 + 2\alpha v^2 \ln(v^2) + \alpha(1 - 2v^2)\ln(1 - v^2)).$$

2) for $0 < v < 0.5$, $-1 - v < \xi < 1 - v$

$$\tilde{F}(\xi,v_{comb}) = \begin{cases} F(\xi,v_{comb}), & -v_{comb} \le \xi < 1 - v_{comb}, \\ \gamma_+ g_1(\xi), & \xi < 1 - v. \end{cases}$$

The constant γ_+ is found from the condition

$$\gamma_+ g''_1(-v_{comb}) = F''(-v_{comb}, -v_{comb}).$$

Here,

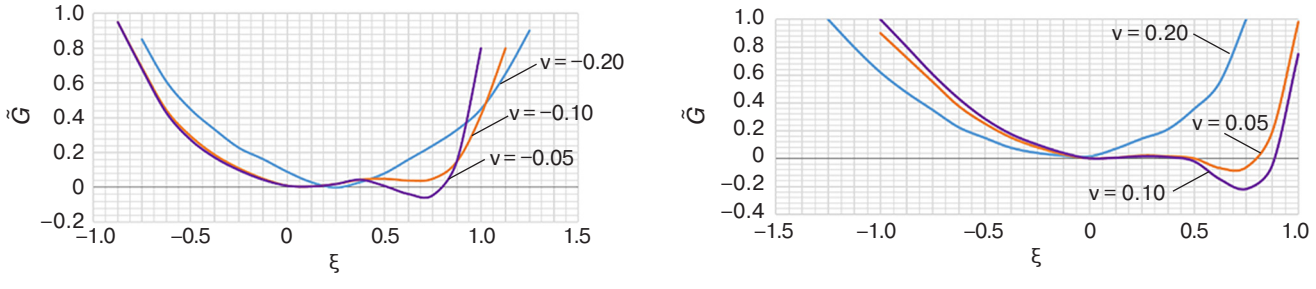
$$g_1(\xi, v) = h^2(1 + \alpha(1 - h^2)^6 \ln(1 - h^2)).$$

The plots of the laminar–turbulent transition potential are shown in Figs. 2a and 2b.

BREAKDOWN EQUATION OF THE LOCAL EQUILIBRIUM MANIFOLD (INSTABILITY OF THE LAMINAR PROCESS OF APPROXIMATION OF LOCAL EQUILIBRIUM)

The work sets out to demonstrate that kinetic energy pumping leads to an excess of energy in the laminar process as the local equilibrium is approached, thus causing its instability. The latter is expressed either by resonance or by breaking out of the local equilibrium manifold, which is characterized by process turbulence. Through the process turbulence, the excess energy generated by the kinetic energy pumping is "dumped." The mathematical model of process turbulence can be described as follows.

In order to simulate the breakdown of the local equilibrium manifold, represented by the breakdown of the laminar combustion process at mixture heating in the



(a) (b)

Fig. 2. Potential $\tilde{F}(\xi; v)$ (a) $v = -0.20, -0.10, -0.05$; (b) $v = 0.05, 0.10, 0.20$

phase space of dimensionless variables $(\tilde{E}, \tilde{u}_1, \tilde{u}_2, \tilde{\rho}, \tilde{T}, \tilde{n})$, it is necessary to move to new variables $(\xi, \tilde{u}_1, \tilde{u}_2, \tilde{\rho}, \tilde{T}, \tilde{n})$, namely, the pumping ξ as a variable of the laminar–turbulent transition. The equations

$$\rho \frac{d}{d\tilde{t}} \tilde{E} + \tilde{P} \widetilde{\operatorname{div}} \tilde{U} = 0; \; (\gamma - 1)\tilde{E} = \xi \tilde{U}^2 \tag{12}$$

allow us to obtain for the pumping:

$$\tilde{\rho}\tilde{U}^2 \frac{d}{d\tilde{t}} \tilde{E} + 2\tilde{\rho}\tilde{U}\xi \frac{d}{d\tilde{t}} \tilde{U} = \tilde{\rho} \frac{d}{d\tilde{t}} (\tilde{U}^2 \xi) = -(\gamma - 1)\tilde{P} \widetilde{\operatorname{div}} \tilde{U},$$

where $\tilde{P}$ is the pressure; $d\tilde{t}$ is the temperature difference.

Hence: $\tilde{\rho} \frac{d}{d\tilde{t}} \xi + \frac{2\tilde{\rho}\xi}{\tilde{U}} \frac{d}{d\tilde{t}} \tilde{U} + \frac{(\gamma - 1)\tilde{P}}{\tilde{U}^2} \widetilde{\operatorname{div}} \tilde{U} = 0.$

Here,

$$\frac{d}{d\tilde{t}} \tilde{U} = \frac{1}{\tilde{\rho}} \frac{d}{d\tilde{t}} (\tilde{\rho}\tilde{U}) - \frac{1}{\tilde{\rho}} \tilde{U} \frac{d}{d\tilde{t}} \tilde{\rho} =$$

$$= \frac{1}{\tilde{\rho}} [-\partial_{\tilde{x}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2^2) - \partial_{\tilde{x}} \tilde{P} + \tilde{\varepsilon}_g (1 - c_0 \tilde{n})\tilde{\rho} -$$

$$- \partial_{\tilde{x}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1^2) - \partial_{\tilde{x}} \tilde{P} + \tilde{\varepsilon}_g c_0 \tilde{n}\tilde{\rho}] + \frac{1}{\tilde{\rho}} \tilde{U} \partial_{\tilde{x}} (\tilde{\rho}\tilde{U}).$$

Finally:

$$\tilde{\rho} \frac{d}{dt} \xi - \frac{2\xi}{\tilde{U}} [\partial_{\tilde{x}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2^2) +$$
$$+ \partial_{\tilde{x}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1^2) + 2\partial_{\tilde{x}} \tilde{P} - \tilde{\varepsilon}_g \tilde{\rho}] +$$
$$+ 2\xi \partial_{\tilde{x}} (\tilde{\rho}\tilde{U}) + \frac{(\gamma - 1)\tilde{P}}{\tilde{U}^2} \widetilde{\operatorname{div}} \tilde{U} = 0.$$

We now regularize the equations of momentum and the equation of continuity (hydrodynamics) by the viscosity:

$$\partial_{\tilde{t}} \tilde{\rho} + \partial_{\tilde{x}} (\tilde{\rho}\tilde{U}) = \tilde{\varepsilon}_R \tilde{\Delta}\tilde{\rho}, \tag{13}$$

$$\partial_{\tilde{t}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2) + \partial_{\tilde{x}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2^2) + \partial_{\tilde{x}} \tilde{P} =$$
$$= \tilde{\varepsilon}_g (1 - c_0 \tilde{n})\tilde{\rho} + \tilde{\varepsilon}_R \tilde{\Delta}\tilde{u}_2,$$

$$\partial_{\tilde{t}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1) + \partial_{\tilde{x}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1^2) + \partial_{\tilde{x}} \tilde{P} =$$
$$= \tilde{\varepsilon}_g c_0 \tilde{n}\tilde{\rho} + \tilde{\varepsilon}_R \tilde{\Delta}\tilde{u}_1,$$

where $\tilde{U} = c_0 \tilde{n}\tilde{U}_1 + (1 - c_0 \tilde{n})\tilde{U}_2$ is the average velocity of the mixture; $\mathrm{Re} = 1 / \tilde{\varepsilon}_R$, $\mathrm{Re} = \eta_D / (U_* L_*) = \eta_D / (\rho_* U_* L_*)$ is the Reynolds number of homogeneous state $\rho_*, n_*, T_*, u_1^*, u_2^*$; η_D is the dynamic viscosity in Reynolds number; $U_* = c_* n_* u_1^* + (1 - c_* n_*)U_*$ is the characteristic velocity of homogeneous mixture; L_* is the characteristic size of the medium; $\tilde{\varepsilon}_R$ is the dynamic viscosity.

From the equation for the internal energy, we derive the equation for the pumping, in which a covariant Cahn diffusion (Cahn operator of variable diffusion) is introduced:

$$\tilde{\rho} \frac{d}{d\tilde{t}} \xi - \frac{2\xi}{\tilde{U}} [\partial_{\tilde{x}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2^2) +$$
$$+ \partial_{\tilde{x}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1^2) + 2\partial_{\tilde{x}} \tilde{P} + \tilde{\varepsilon}_g \tilde{\rho}] +$$
$$+ 2\xi \partial_{\tilde{x}} (\tilde{\rho}\tilde{U}) + \frac{(\gamma - 1)\tilde{P}}{\tilde{U}^2} \widetilde{\operatorname{div}} \tilde{U} = \tag{14}$$
$$= \partial_{\tilde{x}} \left(\frac{\tilde{D}}{\tilde{T}} \partial_{\tilde{x}} (F(\xi, \nu) - \tilde{\varepsilon}_K^2 \partial_{\tilde{x}}^2 \xi) \right),$$

where ε_K is the Cahn alternating diffusion, $\tilde{D} = D / (\rho_* U_* L_* T_*)$, D is the mobility coefficient, and the potential F in this case is $F(\xi, \nu) = \partial_\xi \tilde{G}(\xi, \nu)$.

We add the kinetic equations for temperature and reduced substance $\tilde{n}$. Finally, we obtain a model of vibrational combustion turbulence in hydrodynamics, kinetics, and pumping:

$$\partial_{\tilde{t}} \tilde{\rho} + \partial_{\tilde{x}} (\tilde{\rho}\tilde{U}) = \tilde{\varepsilon}_R \tilde{\Delta}\tilde{\rho}, \tag{15}$$

$$\partial_{\tilde{t}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2) + \partial_{\tilde{x}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2^2) + \partial_{\tilde{x}} \tilde{P} =$$
$$= \tilde{\varepsilon}_g (1 - c_0 \tilde{n})\tilde{\rho} + \tilde{\varepsilon}_R \tilde{\Delta}\tilde{u}_2,$$

$$\partial_{\tilde{t}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1) + \partial_{\tilde{x}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1^2) + \partial_{\tilde{x}} \tilde{P} =$$
$$= \tilde{\varepsilon}_g c_0 \tilde{n}\tilde{\rho} + \tilde{\varepsilon}_R \tilde{\Delta}\tilde{u}_1,$$

$$\tilde{\rho}\tilde{c} \frac{d}{d\tilde{t}} \tilde{T} = \partial_{\tilde{x}} (\tilde{\lambda} \partial_{\tilde{x}} \tilde{T}) + \tilde{T}\tilde{S}\tilde{W}(\tilde{n}, \tilde{T}), \tag{16}$$

$$\tilde{\rho} \frac{d}{d\tilde{t}} \tilde{n} = \partial_{\tilde{x}} (\tilde{\rho}\tilde{D} \partial_{\tilde{x}} \tilde{n}) - \tilde{W}(\tilde{n}, \tilde{T}),$$

$$\tilde{W} = \tilde{k}_0 \tilde{\rho}\tilde{n}^\beta \mathrm{e}^{-\frac{\tilde{E}_*}{RT}}, \tag{17}$$

$$\tilde{\rho} \frac{d}{d\tilde{t}} \xi - \frac{2\xi}{\tilde{U}} [\partial_{\tilde{x}} ((1 - c_0 \tilde{n})\tilde{\rho}\tilde{u}_2^2) +$$
$$+ \partial_{\tilde{x}} (c_0 \tilde{n}\tilde{\rho}\tilde{u}_1^2) + 2\partial_{\tilde{x}} \tilde{P} + \tilde{\varepsilon}_g \tilde{\rho}] + 2\xi \partial_{\tilde{x}} (\tilde{\rho}\tilde{U}) + \tag{18}$$
$$+ \frac{(\gamma - 1)\tilde{P}}{\tilde{U}^2} \widetilde{\operatorname{div}} \tilde{U} = \partial_{\tilde{x}} \left(\frac{\tilde{D}}{\tilde{T}} \partial_{\tilde{x}} [\hat{F}(\xi, \nu) - \hat{\varepsilon}_K^2 \partial_{\tilde{x}}^2 \xi] \right),$$

$$\tilde{P} = \tilde{P}_{\text{ad,g}} + \tilde{P}_{\text{comb}} + \left(-\tilde{T}\frac{d\tilde{\mu}_0(\tilde{T})}{d\tilde{T}} + \tilde{\mu}_0(\tilde{T}) \right)\tilde{n}\tilde{\rho}, \quad (19)$$

$$\tilde{S} = -\left(\frac{d}{d\tilde{T}}\tilde{\mu}_0(\tilde{T}) + \ln\left(\frac{\tilde{\rho}^2\tilde{T}\tilde{n}}{\tilde{\rho}_0^2\tilde{T}_0\tilde{n}_0} \right) \right)\tilde{n}.$$

NUMERICAL EXPERIMENT OF THE MODEL (15)–(19)

In order to establish the possibility of combustion turbulence, we perform numerical experiments of model (15)–(19) on a segment $\tilde{x} \in [0,1]$ with boundary conditions to control the kinetic energy pumping rate:

$$\tilde{u}_2|_{\tilde{x}=0} = \tilde{u}_2^0(1+V\tilde{t})\partial_{\tilde{x}}\tilde{\rho}|_{\tilde{x}=0} = \partial_{\tilde{x}}\tilde{\rho}|_{\tilde{x}=1} =$$
$$= \partial_{\tilde{x}}\tilde{u}_1|_{\tilde{x}=0} = \partial_{\tilde{x}}\tilde{u}_1|_{\tilde{x}=1} = \partial_{\tilde{x}}\tilde{T}|_{\tilde{x}=0} = \partial_{\tilde{x}}\tilde{T}|_{\tilde{x}=1} = 0,$$
$$\partial_{\tilde{x}}\tilde{u}_2|_{\tilde{x}=1} = \partial_{\tilde{x}}\tilde{n}|_{\tilde{x}=0} = \partial_{\tilde{x}}\tilde{n}|_{\tilde{x}=1} = 0,$$
$$\partial_x\xi|_{x=0} = \partial_x\xi|_{x=1} = \partial_x\mu|_{x=0} = \partial_x\mu|_{x=1},$$

(where $\mu = \hat{F}_{\text{comb}}(\xi,\nu) - \hat{\varepsilon}_{\text{K}}^2\partial_{\tilde{x}}^2\xi$, $\hat{F}_{\text{comb}}$ is the free energy resulting from the calculation) and initial conditions modeling, in the one-dimensional case, the injection from the nozzle of the combustible component of a two-component mixture:

$$\tilde{\rho}|_{\tilde{t}=0} = \tilde{\rho}_0 = 1,\ \tilde{u}_1|_{\tilde{t}=0} = \tilde{u}_1^0 = 0.2,$$
$$\tilde{u}_2|_{\tilde{t}=0} = \tilde{u}_2^0 = 0.2,\ \tilde{T}|_{\tilde{t}=0} = \tilde{T}_0 = 10,$$

$\tilde{E}_* = 100$. Initial data for pumping ξ_0 = const from the lability zone of the potential $\hat{F}_{\text{comb}}(\xi,\nu_\upsilon)$ (index υ is the velocity turbulence) is:

$$\tilde{\varepsilon}_{\text{K}} = 0.04,\ \tilde{\varepsilon}_{\text{g}} = 0.01.$$

Example 1 (Figs. 3a–3h). The resonance elimination by turbulence (far from resonance), for $j = 1$ in the standard chemical potential formula:

$$\tilde{\mu}_0(\tilde{T}) = \tilde{T}_0\left[B_* - (R + A_*)\frac{\tilde{T}^j}{\tilde{T}_0^j} \right], \quad (20)$$

where $\tilde{\mu}_0(\tilde{T})$ is the chemical potential; $\tilde{T}_0$ is the initial temperature; $\tilde{T}, B_*, A_*$ are constants; and R is the universal gas constant.

The basic turbulence parameters for vibrational combustion are $u_1(0) = u_2(0) = 10$, $\xi(0) = 0.2$, $\rho(0) = 1$. The cross sections in all the plots below are $t = 0.005$, 0.01, 0.025, 0.035, 0.05, 0.065, 0.125; $T(0) = 10$.

As can be seen in Fig. 3a and 3b, the pressure increases and the entropy decreases, i.e., deflagration becomes detonation when turbulence is involved. There is an increase in temperature and density.

Example 2 (Figs. 4a–4j). The resonance elimination by turbulence (for critical values $A_* + R = 3$), for $j = 4$ in (20). We consider the account for the basic turbulence parameters of vibrational combustion: $u_1(0) = u_2(0) = 10$, $\xi(0) = 0.2$, $\rho(0) = 1.5$. For all plots below the cross-section $t = 0$, 0.005, 0.010, 0.025, 0.035, 0.050, 0.065, 0.125. The first case (base case): $T(0) = 5$. The pressure and the entropy increase significantly. There is a wide zone of the detonation mode of the vibrational combustion (in the absence of turbulence, there was a narrow zone of the detonation combustion close to the resonance [3]). The internal energy increases but decreases relative to pumped kinetic energy $\xi \to 0$. A part of the pumped kinetic energy is converted into heat.

Example 3 (Figs. 5a–5j). The resonance elimination for $j = 4$ (20) (far from the critical resonance parameters), at low temperatures, with the basic turbulence parameters $u_1(0) = u_2(0) = 12$, $\xi(0) = 0.2$, $\rho(0) = 1.5$, and the cross-section $\tilde{t} = 0$, 0.005, 0.010, 0.025, 0.035, 0.050, 0.065, 0.125. Here, $T(0) = 0.8$. The pressure and the entropy decrease. The internal energy increases but decreases relative to pumped kinetic energy $\xi \to 0$. A part of the kinetic energy is converted into heat ($\tilde{T}$ and $\tilde{T}\tilde{S}$ increase).

Example 4 (Figs. 6a–6j). The resonance elimination by turbulence (close to the critical resonance parameters) for $j = 4$ in (20), at low temperatures, $u_1(0) = u_2(0) = 8$, $\xi(0) = 0.2$, $\rho(0) = 1.5$, cross-section $\tilde{t} = 0$, 0.005, 0.010, 0.025, 0.035, 0.050, 0.065, 0.125; $T(0) = 0.8$.

The entropy decreases and the pressure increases (the same as before turbulence, but the detonation zone is much wider). The internal energy increases but decreases relative to pumped kinetic energy ($\xi \to 0$). A part of the pumped kinetic energy is converted into heat (the internal energy $\tilde{E}$ and $\tilde{T}$ increase).

Example 5 (Figs. 7a–7j). Mixing. Numerical experiment (20) for $j = 4$, $A_* + R = 0.5$ (base parameters); $\tilde{\text{n}}|_{\tilde{t}=0} = \tilde{\text{n}}_0 = 1$, $\tilde{u}_1|_{\tilde{t}=0} = \tilde{u}_1^0 = 0.2$; $\tilde{u}_2|_{\tilde{t}=0} = \tilde{u}_2^0 = 0.2$; $\tilde{T}|_{\tilde{t}=0} = \tilde{T}_0 = 10$ are constants; $\tilde{n}|_{\tilde{t}=0} = \tilde{n}_1 = 0.5$, $\tilde{x} \in (0;0.3) \cup (0.4;0.5)$, $\tilde{n}|_{\tilde{t}=0} = 0.66$, $\tilde{x} \in (0.3;0.4)$; $E_* = 100$; $\tilde{t} = 0$, 0.005, 0.010, 0.025, 0.035, 0.050, 0.065, 0.125; initial data for internal energy $\tilde{E}_0 = \text{const}$, $\tilde{T}_0 = 8$, $\tilde{u}_2 = 8$.

Resonance elimination for mixing. Modeling the injection of the combustible component of a two-component mixture from three nozzles in the one-dimensional case with initial conditions.

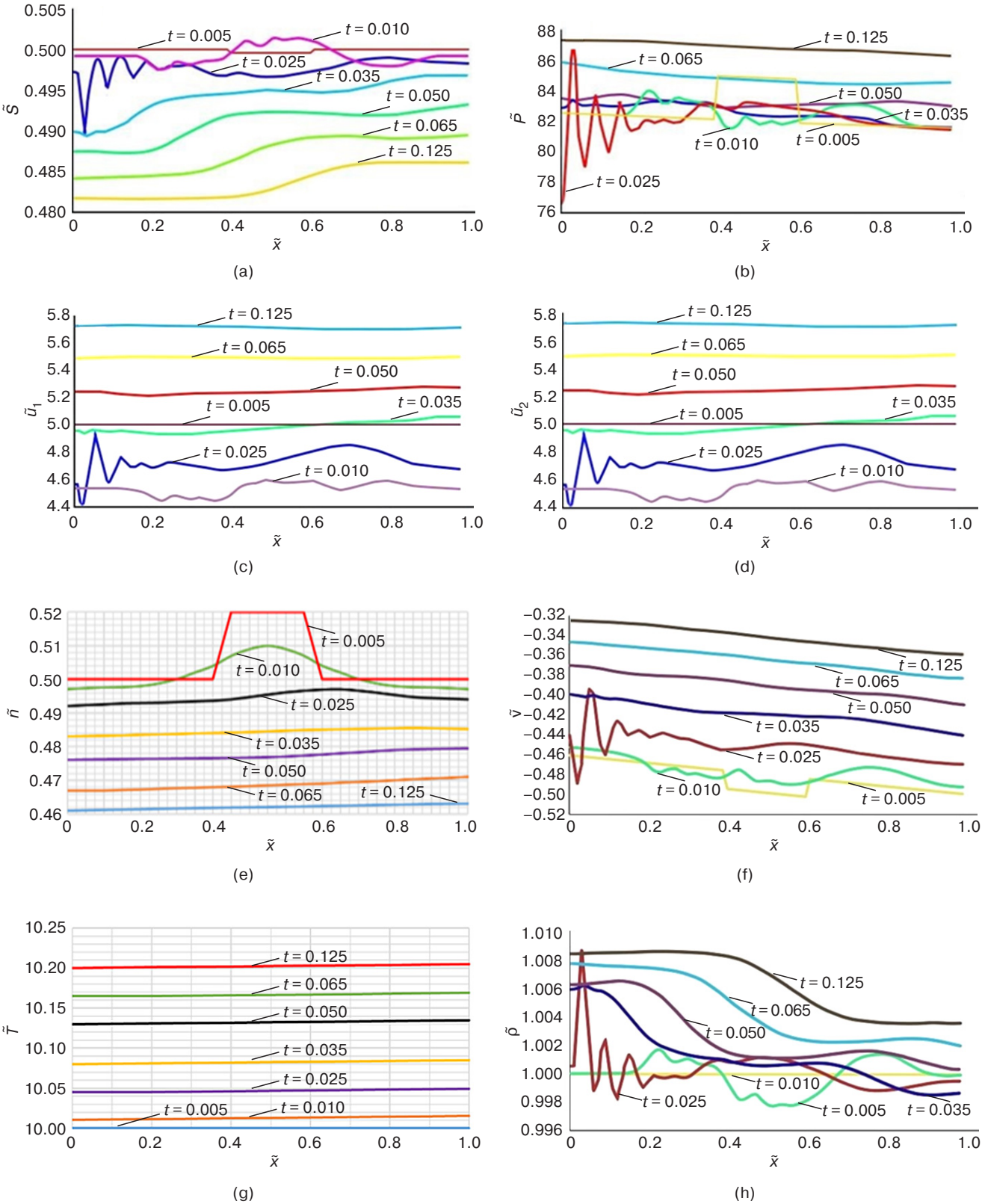


Fig. 3. Numerical experimental results of model (15)–(19) on the segment $\tilde{x} \in [0,1]$ for different t: (a) $\tilde{S}$; (b) $\tilde{P}$; (c) $\tilde{u}_1$; (d) $\tilde{u}_2$; (e) reduced amount of substance $\tilde{n}$; (f) $\tilde{v}$; (g) $\tilde{T}$; (h) $\tilde{\rho}$

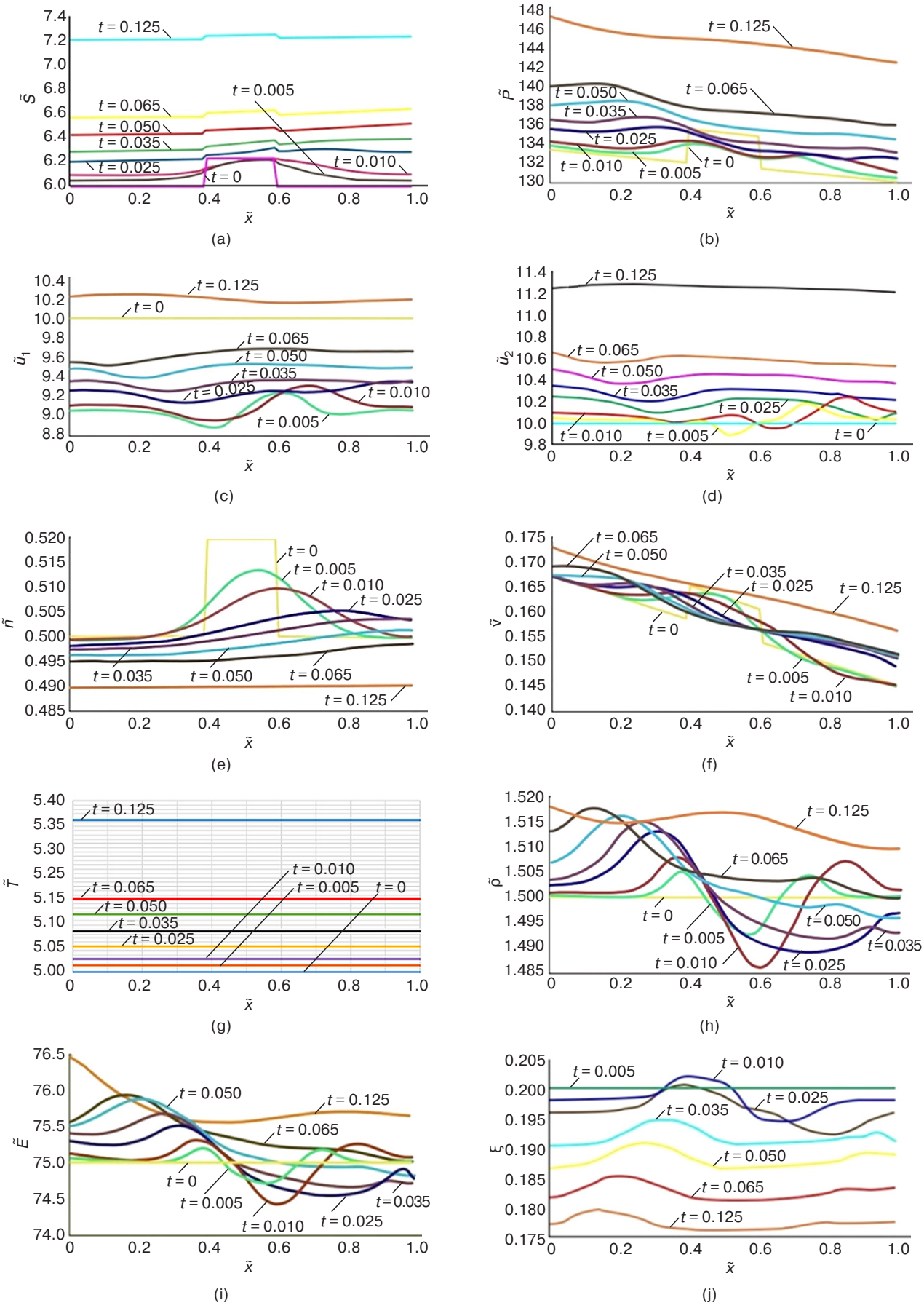


Fig. 4. Calculation results for the basic turbulence parameters of vibrational combustion for different t: (a) $\tilde{S}$; (b) $\tilde{P}$; (c) $\tilde{u}_1$; (d) $\tilde{u}_2$; (e) $\tilde{n}$; (f) $\tilde{v}$; (g) $\tilde{T}$; (h) $\tilde{\rho}$; (i) $\tilde{E}$; (j) ξ

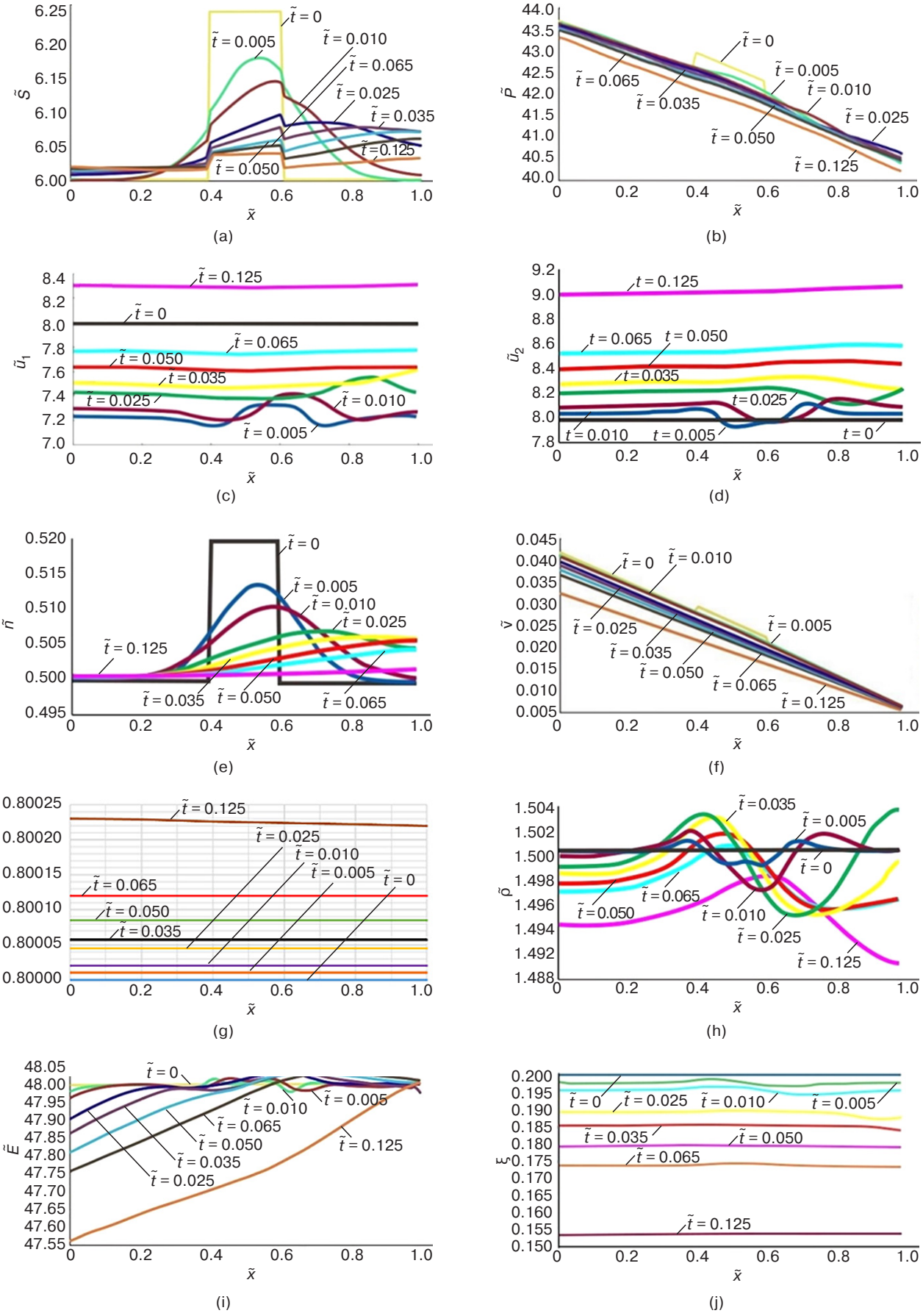


Fig. 5. Calculation results of the resonance elimination for $j = 4$ (20) (far from the critical resonance parameters) at low temperatures for different $\tilde{t}$: (a) $\tilde{S}$; (b) $\tilde{P}$; (c) $\tilde{u}_1$; (d) $\tilde{u}_2$; (e) $\tilde{n}$; (f) $\tilde{v}$; (g) $\tilde{T}$; (h) $\tilde{\rho}$; (i) $\tilde{E}$; (j) ξ

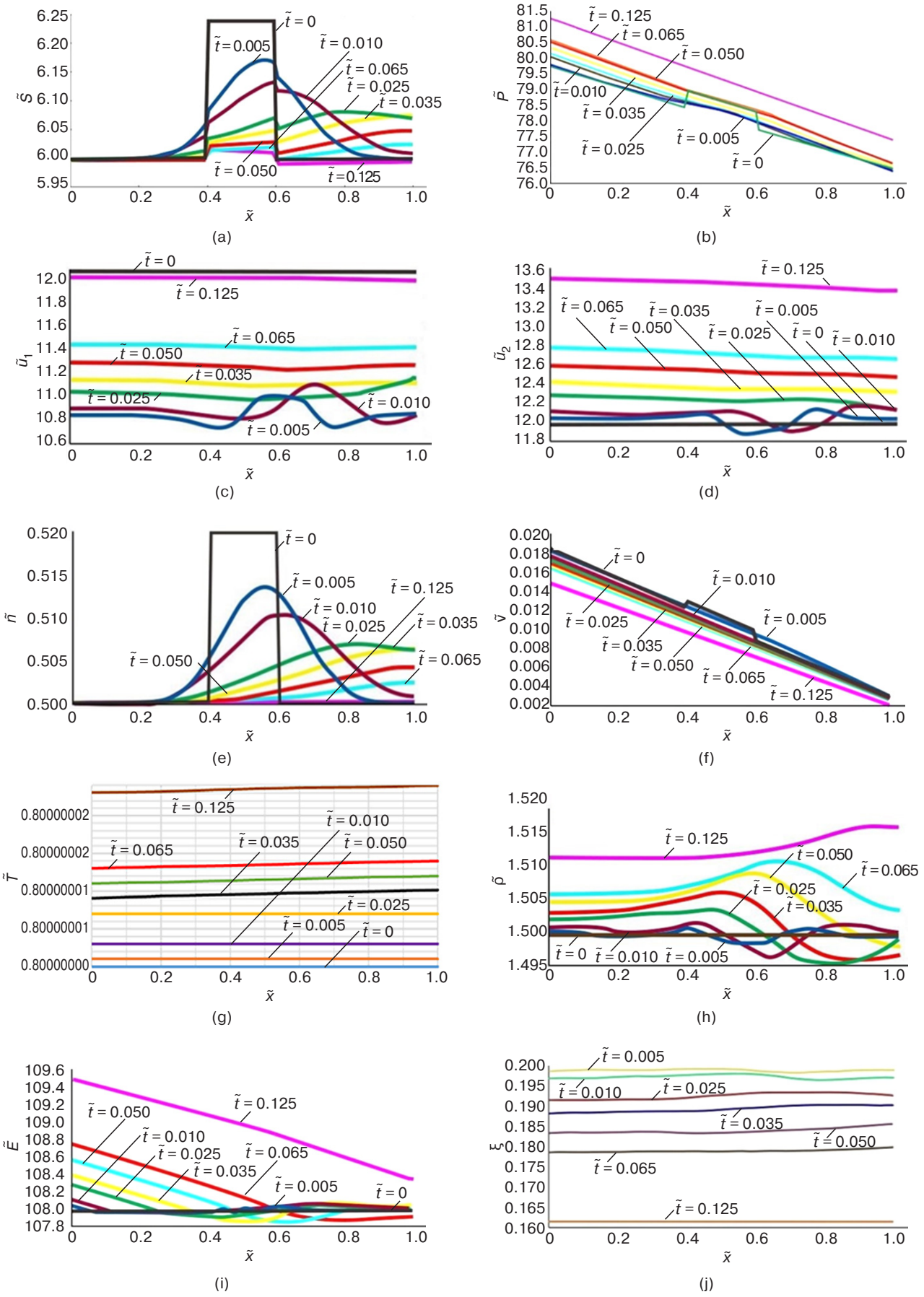


Fig. 6. Calculation results for the resonance elimination by turbulence (close to the critical resonance parameters) for $j = 4$ in (20) at low temperatures for different $\tilde{t}$: (a) $\tilde{S}$; (b) $\tilde{P}$; (c) $\tilde{u}_1$; (d) $\tilde{u}_2$; (e) $\tilde{n}$; (f) $\tilde{v}$; (g) $\tilde{T}$; (h) $\tilde{\rho}$; (i) $\tilde{E}$; (j) ξ

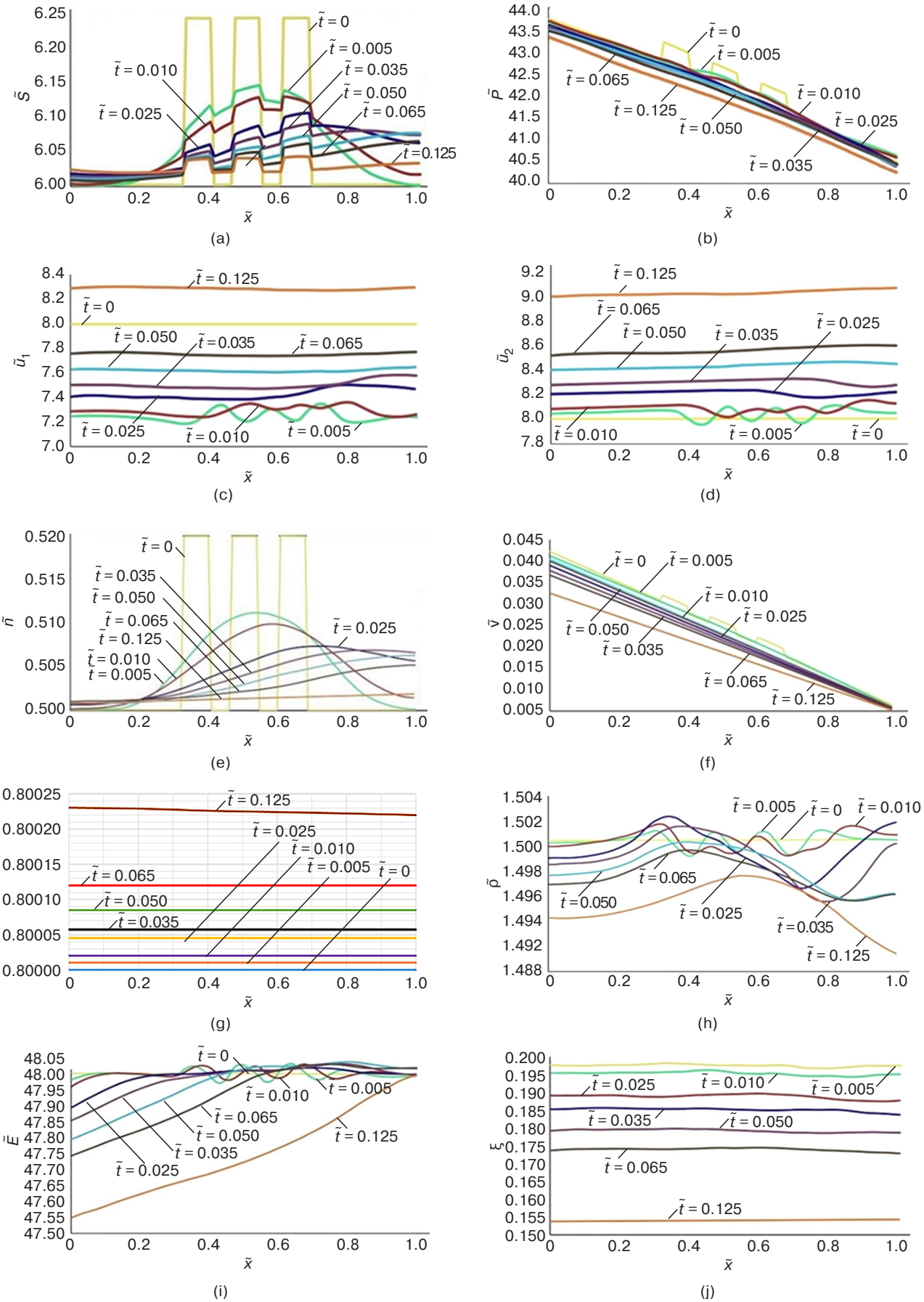


Fig. 7. Numerical results of the experiment (20) for $j = 4$, $A_* + R = 0.5$ for different $\tilde{t}$: (a) $\tilde{S}$; (b) $\tilde{P}$; (c) $\tilde{u}_1$; (d) $\tilde{u}_2$; (e) $\tilde{n}$; (f) $\tilde{v}$; (g) $\tilde{T}$; (h) $\tilde{\rho}$; (g) $\tilde{E}$; (j) ξ

The entropy and the pressure continue to decrease (as before turbulence). However, as the velocity $\tilde{u}^2$ of the neutral component at the input increases, detonation combustion mode occurs. The numerical experiment also predicts a detonation combustion mode. Meanwhile, temperature, density, and internal energy increase. The pattern of the plots reflects the effect of gravity. Similar numerical experimental results are obtained for resonance elimination by turbulence $j = 4$ in (20) under mixing, with an increase in the initial velocity of the passive variable $\tilde{u}_2^0 = 10$. As the velocity of the neutral component $\tilde{u}_2$ at the input increases with mixing, the detonation combustion mode occurs.

CONCLUSIONS

The described studies support the conclusion that the thermodynamic method offers fundamental possibilities for studying the evolution of a system (in this case, the tendency of stratification into "turbulent" and "non-turbulent" combustion). It should be noted that the applied thermodynamic analysis can only indicate process evolution trends (main possibility of implementation) and the choice of system evolution trajectory, but not the speed of this process. The analysis confirms that regions of laminar combustion stability develop during combustion, along with metastable and labile regions where laminar combustion is unstable. However, this does not imply that there will be no signs of turbulence in the developed state of the region of stability. The diffusion of perturbations in these regions will dilute them, while in the regions of instability the process of "negative" (Cahn) diffusion will concentrate them. It can be assumed that regions of instability of the homogeneous system are sources of perturbations, and regions of stability are sinks. These assumptions have been verified by numerical experiments using the mathematical model described above. When starting from the initial thermodynamic model, the mathematical model of the laminar–turbulent transition during the combustion as an analog of the nonequilibrium phase transition can become complicated.

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Authors' contributions

E.V. Radkevich—development and mathematical interpretation of the combustion model.

M.E. Stavrovsky—description of models of critical phenomena.

O.A. Vasilyeva—numerical experiment of models.

N.N. Yakovlev—full-scale experiment, obtaining data for models.

M.I. Sidorov—verification of the adequacy of models and description of processes.

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