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INFLUENCE OF TURBULENCE ON THE FORMATION OF DETONATION COMBUSTION OF A GAS IN TUBES

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Conditions for transition of the slow combustion of a gas to detonation are determined based on the solution of the problem on propagation of turbulent combustion initiated at the end wall of a semiinfinite tube. The combustion zone is modeled by an infinitely thin flame front. It is assumed that the turbulence develops ahead of the flame in the flow behind the shock wave formed. Simplified Reynolds equations underlie a mathematical description of turbulent flow. The assumptions made of the local isotropy of turbulence in the flow core and the hypotheses for the generation and dissipation of pulsation energy make it possible to close the considered system of equations in the one-dimensional case.

Introduction. The ignition of the gas at the end wall of a semiinfinite tube causes the flame to propagate and the leading shock wave to appear (see, e.g., [1]). For fairly large Reynolds numbers, the gas flow formed behind this wave becomes turbulent. Turbulence generated on the walls is mainly responsible for the acceleration of flames in tubes [2]. To describe the turbulence one uses Navier–Stokes equations or different turbulence models enabling one to close Reynolds equations whose solution is a difficult problem. Also, investigation of the processes of combustion of gas mixtures involves consideration of rather complex (nonequilibrium, as a rule) chemical transformations. Therefore, the problem of modeling of turbulent combustion, in particular, of slow combustion-to-detonation transition, remains topical.

In this work, we propose a series of simplifications that makes it possible to solve the problem on the possibility of combustion-to-detonation transition in a one-dimensional formulation.

Two-Phase Approximation of Turbulent Flows. The Reynolds method provides a practical basis for modeling developed turbulent flows at present. The value of any parameter is represented in the form of the sum of its average value on a certain time interval and the pulsating component which is assumed to be small compared to the corresponding average value [3]: $\Psi = \bar{\Psi} + \Psi'$, $|\Psi'| << |\bar{\Psi}|$. Here and in what follows an overbar means time averaging in accordance with the existing rules [4, 5].

Unlike the traditional procedure of derivation of Reynolds equations, in the present work, we propose that the turbulent flow be considered as flow of a two-phase medium. The density, the velocity vector, the internal energy, and the pressure of one, "basic," phase are prescribed by the quantities $\bar{\rho}$, $\mathbf{u}$, e, $p_1 = \bar{p} + p'$, where $\bar{p} = \bar{\rho}\bar{e}(\gamma - 1)$ and $p' = \bar{\rho}e'(\gamma - 1)$; for the other phase the corresponding role is played by the quantities p', $\bar{\mathbf{u}}$, e, and $p_2 = \rho' e(\gamma - 1)$. This second phase can be called "fictitious," since it is absent from the averaged motion: $\bar{\rho}' = 0$. It would appear natural that the contribution of the "fictitious" phase to the averaged values of the mass, momentum, and energy fluxes is negligible, too. Then we can disregard terms with a cofactor ρ' in the initial Navier–Stokes equations. As a result of the averaging of the equations belonging just to the "basic" phase, the Reynolds equations, for a constant value of the adiabatic exponent γ, take the form

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \overline{\rho u_j}}{\partial x_j} = 0\,, \quad \frac{\partial \overline{\rho u_i}}{\partial t} + \frac{\partial \overline{\rho u_i u_j}}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial \bar{R}_{ij}}{\partial x_j}\,,$$

$$\frac{\partial \bar{\rho}\left(\bar{e} + e_{\mathrm{v}} + \bar{\mathbf{u}}^2/2\right)}{\partial t} + \frac{\partial \overline{\rho u_j}\left(\bar{h} + e_{\mathrm{v}} + \bar{\mathbf{u}}^2/2\right)}{\partial x_j} = \tag{1}$$

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$$= \bar{A}_\mu + \bar{A}_\tau - \frac{\partial\left(\bar{Q}_{\lambda j} + \bar{Q}_{\tau j}\right)}{\partial x_j} + A_{\tau'}, \quad \bar{p} = \bar{e}\,(\gamma - 1)\,\bar{\rho}, \quad \bar{h} = \bar{e} + \bar{p}/\bar{\rho}.$$

Here $\bar{R}_{ij} = -\bar{\rho}\overline{u'_i u'_j}$, $\bar{A}_\mu = \partial\bar{\rho}\,\bar{u}_i\,\bar{\tau}_{ij}/\partial x_j$, $\bar{A}_\tau = \partial\bar{\rho}\,\bar{u}_i\,\bar{R}_{ij}/\partial x_j$, $\bar{Q}_{\tau j} = \bar{\rho}\,\overline{u'_j h'}$, $A_{\tau'} = \partial\overline{u'_i \tau'_{ij}}/\partial x_j$, and $e_v = \overline{u'_i u'_i}/2 = |\mathbf{u}'|^2/2$. There are no such undetermined quantities as $\rho' u'_j$ and $\rho' e'$ in these equations of "two-phase" approximation, but, at the same time, they contain all substantial terms having a clear physical meaning. The recurrence of the subscript i or j here and in what follows means summation over it.

For a constant coefficient of molecular viscosity μ_*, the tensors τ'_{ij} and s'_{ij} are determined by the same relations as the corresponding tensors of viscous stresses and strain rates in the Navier–Stokes equations but are dependent on the fluctuations of the total rate $\tau'_{ij} = 2\mu_*(s'_{ij} - \delta_{ij}\ \mathrm{div}\ (\mathbf{u}')/3)$ and $s'_{ij} = (\partial u'_i/\partial x_j + \partial u'_j/\partial x_i)/2$ rather than on the total rate.

With account for the expressions for τ'_{ij} and s'_{ij}, the work of viscous-stress pulsations is prescribed by the expression

$$A_{\tau'} = \frac{\partial\overline{u'_i \tau'_{ij}}}{\partial x_j} = \frac{1}{2}\frac{\partial\mu_*\partial\overline{u'_i u'_i}/\partial x_j}{\partial x_j} + \frac{\partial\mu_*\partial\overline{u'_i u'_i}/\partial x_j}{\partial x_j} - \frac{5}{3}\frac{\partial\mu_*\overline{u'_j \mathrm{div}\,(\mathbf{u}')}}{\partial x_j}. \tag{2}$$

It should be noted that Eqs. (1) can also be obtained by strict averaging of the total Navier–Stokes equations over time without prediscarding terms with a factor ρ'. For this purpose we need only disregard the correlation terms of third order and take into account that $|\rho'\mathbf{u}'| << |\bar{\rho}\,\bar{\mathbf{u}}|$ and $|\rho' e'| << \bar{\rho}\,\bar{e}$.

Using the well-known procedure presented, e.g., in [3], for the pulsation energy e_v in the same approximation we easily obtain the equation

$$\bar{\rho}\frac{de_v}{dt} = \bar{R}_{ij}\bar{s}_{ij} - \overline{\tau'_{ij}s'_{ij}} + A_{\tau'}. \tag{3}$$

Unlike the work of internal surface forces due to molecular viscosity [4], the quantity $\bar{R}_{ij}\bar{s}_{ij}$ determines in the general case neither the generation nor dissipation of pulsation energy, since the tensor $\bar{R}_{ij}$ is related to the tensor of strain rates $\bar{s}_{ij}$ of the averaged flow not in the same manner as the viscous-stress tensor τ_{ij}. The term $\tau'_{ij}\,s'_{ij} > 0$ describes the dissipation of pulsation energy.

Model of Vibrating Liquid Particles. Turbulent flow can be considered as a flow of turbulent vortices moving relative to the averaged flow [3]. At each instant of time, the parameters at any point become equal to the values brought here together with the coming turbulent vortices. During the period of averaging, the vortices at the distance $r' = |\Delta\mathbf{r}|$ which is covered by them over a period shorter than the period of averaging can reside at a point prescribed by the vector $\mathbf{r}$. At the same time, in the "two-phase" approximation in question, a continuity equation for the fictitious phase has the form

$$\frac{\partial\rho'}{\partial t} + \frac{\partial\rho'\,(\bar{u}_j + u'_j)}{\partial x_j} = 0.$$

Hence with allowance for the corresponding equations for the averaged and actual flows we can obtain the condition

$$\frac{\partial\bar{\rho}u'_j}{\partial x_j} = 0, \tag{4}$$

which means that the mass of any gas particle of the averaged flow is not altered by the medium's pulsations. The nature of the term e_v in the energy equation of the averaged flow and condition (4) enable us to model the random movement of turbulent vortices arriving at a prescribed point of the flow by the oscillation of a liquid particle with a density $\bar{\rho}$ about this point. The quantities e_v and $W = \sqrt{\overline{u'_i u'_i}} = |\overline{u'}|$ can be interpreted as the average pulsation energy

and the average modulus of velocity of these oscillations; here, we have $e_v = W^2/2$. The force keeping vibrating liquid particles from penetrating into the averaged flow is determined by the vector $\mathbf{f} = 0.5n\bar{\rho}C_*S|\mathbf{u}'|\mathbf{u}'$ by analogy with two-phase media. If l is the average dimension of a vortex, the number of vortices per unit volume is $n \approx l^{-3}$ and the cross-sectional area of a vortex is $S \approx l^2$. The kinetic energy of oscillating vortices is expended in overcoming the resistance from the averaged flow. Therefore, the dissipation of pulsation energy can be evaluated by the work of "interphase-friction" force $\tau'_{ij}s'_{ij} = \mathbf{u}'\mathbf{f}$. For small Reynolds number Re_* of oscillatory motion, we have the estimate [6] $C_* \approx 20/\mathrm{Re}_* \approx 20\mu_*/(\bar{\rho}|\mathbf{u}'|l)$ for the resistance coefficient. Thus, the rate of dissipation of pulsation energy per unit volume is represented in the form

$$\overline{\tau'_{ij}s'_{ij}} = \overline{u'_i f_i} \approx 10\mu_*\overline{u'_l u'_l}/l^2 = 10\mu_* W^2/l^2 = 20\mu_* e_v/l^2 . \tag{5}$$

The fluctuation of the enthalpy h' in the energy equation of the averaged flow can be interpreted as the difference of the averaged values at the points $\mathbf{r}$ and $\mathbf{r} + \Delta\mathbf{r}$. If we introduce temperature by a relation characteristic of an ideal gas, i.e., take that $T_g = R_0 p(\mu\bar{\rho})^{-1}$, we can evaluate the quantity h', using the Prandtl representation $h' \approx c_p(T_g(\mathbf{r} + \Delta\mathbf{r}) - \bar{T}_g(\mathbf{r}))$. Then the turbulent heat flux will be determined by the relation

$$\bar{Q}_{\tau j} = \bar{\rho}\overline{u'_j h'} \approx \bar{\rho}c_p\overline{u'_j r'}\frac{\partial \bar{T}_g}{\partial \mathbf{r}} = -\bar{\rho}c_p\overline{|\mathbf{u}'|\, u'_{\mathrm{un}j} r'}\frac{\partial \bar{T}_g}{\partial x_i}u'_{\mathrm{un}i} = -\lambda_{ij}\frac{\partial \bar{T}_g}{\partial x_i}, \tag{6}$$

which is a generalization of the Prandtl formula. Here $u'_{\mathrm{un}j}$ are the components of the unit vector of pulsation velocity $\mathbf{u}'_{\mathrm{un}} = \mathbf{u}'/|\mathbf{u}'|$ and $\lambda_{ij} = \bar{\rho}c_p\overline{|\mathbf{u}'|\, r'\, u'_{\mathrm{un}i}\, u'_{\mathrm{un}j}}$. Thus, the vector of turbulent thermal conductivity in the general case is determined by the gradient of the averaged temperature and the tensor of turbulent-thermal-conductivity coefficients. In deriving (6), we use the apparent relations $\partial/\partial\mathbf{r} = \cos\varphi_j\partial/\partial x_j$ and $\cos\varphi_j = -u'_{\mathrm{un}j}$.

The work of viscous-stress pulsations (2) with account for (4) is reduced to the form

$$A_{\tau'} = \frac{\partial\overline{u'_i\tau'_{ij}}}{\partial x_j} = \frac{\partial\nu_*\bar{\rho}\partial e_v/\partial x_j}{\partial x_j} + \frac{\partial\nu_*\bar{\rho}\partial\overline{u'_i u'_j}/\partial x_i}{\partial x_j} + \frac{5}{3}\frac{\partial\nu_*\overline{u'_i u'_j}\,\partial\bar{\rho}/\partial x_i}{\partial x_j}. \tag{7}$$

Approximation of Locally Isotropic Turbulence. In the flow core, all directions are equally probable for vibrations of averaged-flow particles, i.e., each direction is realized with equal frequency during the averaging period T, and the value of the pulsation-velocity modulus is independent of the direction of pulsations. The unit vector of pulsation velocity is represented in the form $\mathbf{u}'_{\mathrm{un}} = \mathbf{u}'/|\mathbf{u}'| = (u'_{\mathrm{un}1}, u'_{\mathrm{un}2}, u'_{\mathrm{un}3}) = (\sin\theta\cos\alpha, \sin\theta\sin\alpha, \cos\theta)$, whereas the averaged product of its components is represented as

$$\overline{u'_l u'_j} = \frac{1}{T}\int_0^T \overline{|\mathbf{u}'|^2}\, u'_{\mathrm{un}i}u'_{\mathrm{un}j}dt = W^2 I_{ij}, \quad I_{ij} = \overline{u'_{\mathrm{un}i}u'_{\mathrm{un}j}} = \frac{1}{T}\int_0^T u'_{\mathrm{un}i}u'_{\mathrm{un}j}dt .$$

By virtue of the equal probability of all directions, the time dt of residence of the end of the vector $\mathbf{u}'_{\mathrm{un}}$ on the surface element of the sphere of unit radius is in proportion to the area of this element $d\Omega = \sin\theta d\theta d\alpha$. The averaging period T corresponds to the total surface area of the sphere of unit radius; therefore, we have $dt = Td\Omega/4\pi = T\sin\theta\, d\theta d\alpha/4\pi$. Then the correlation factor is determined by the integral over the total surface of the unit sphere $I_{ij} = \frac{1}{T}\int_0^T u'_{\mathrm{un}i}\,u'_{\mathrm{un}j}\,dt = \frac{1}{4\pi}\int_0^{4\pi} u'_{\mathrm{un}i}\,u'_{\mathrm{un}j}\,d\Omega = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} u'_{\mathrm{un}i}\,u'_{\mathrm{un}j}\,\sin\theta\, d\theta d\alpha$. Performing reintegration with allowance for the expressions for the components of the unit vector $\mathbf{u}'_{\mathrm{un}}$, we easily obtain $I_{ij} = \delta_{ij}/3$. The Reynolds-stress tensor in this case is reduced to the form $\bar{R}_{ij} = -\bar{\rho}W^2\delta_{ij}/3$.

Under local-isotropy conditions, the path of turbulent vortices r' is dependent just on the modulus of pulsation velocity and is direction-independent; therefore, the tensor of turbulent-thermal-conductivity coefficients is determined by a single scalar quantity $\lambda_{ij} = \overline{\rho} c_p |\mathbf{u}'| r' u'_{un} u'_{un} = \lambda_\tau \delta_{ij}$, $\lambda_\tau = \overline{\rho} c_p |\mathbf{u}'| r'/3 = \overline{\rho} c_p W L_*/3$. Here the quantity $L_* = |\mathbf{u}'| r'/W$ has the dimension of length and determines the average distance at which the influence of turbulence is manifested in the formation of the average flow parameters at a prescribed point $\mathbf{r}$. Therefore, we can consider L_* as the full scale of turbulence. If we introduce the components of the full scale $L = L_*/\sqrt{3}$ and the pulsation velocity in one direction $V^2 = u_1' u_1' = u_2' u_2' = u_3' u_3' = W^2/3$, for the components of the turbulent heat flux (6), we easily obtain the expression

$$\overline{Q}_{\tau j} = -\lambda_\tau \partial \overline{T}/\partial x_j\,, \quad \lambda_\tau = \overline{\rho}\,(c_p - R_0/\mu)\, WL_*/3 = \overline{\rho}\,(c_p - R_0/\mu)\, VL\,. \tag{8}$$

Under the conditions in question, the work of viscous-stress pulsations (7) is prescribed by the relation

$$A_{\tau'} = \frac{5}{9}\frac{\partial \nu_* \overline{\rho} \partial e_v/\partial x_j}{\partial x_j} + \frac{10}{9}\frac{\partial \nu_* \partial \overline{\rho} e_v/\partial x_j}{\partial x_j}\,. \tag{9}$$

Thus, this quantity describes the diffusion of the mass e_v and bulk $\overline{\rho} e_v$ densities of pulsation energy. The diffusion coefficients are determined by the molecular viscosity of the gas.

One-Dimensional Approximation for Turbulent Flows in Channels. The conditions of locally isotropic turbulence hold true only in the flow core. The turbulent boundary layer represents the anisotropic region of flow [3]. The presence of the walls leads to a broken local isotropy at a distance smaller than the turbulence scale. Therefore, it can be assumed that the thickness of the turbulent boundary layer Δ is of the order of the turbulence scale: $\Delta \approx L$. However, the idea exists that the anisotropy is substantially pronounced only in the interior of the boundary layer where pulsations are mainly generated [5]. The thickness of this part of the turbulent boundary layer δ amounts to about 20% of the thickness of the entire layer Δ [5], i.e., $\delta \approx 0.2\Delta$. Therefore, when a one-dimensional approximation is formulated, it is assumed that the turbulent flow is locally isotropic over the entire cross section of the tube, and the influence of the walls and the interior of the boundary layer is allowed for by introducing the source terms characterizing the friction on the walls f_w and the generation of pulsations J into the equations of motion and pulsation energy. If the viscous stresses and molecular heat fluxes in the averaged flow are assumed to be negligible compared to the corresponding turbulent quantities and the diffusion of pulsation energy A'_τ is disregarded compared to its generation, Eqs. (1) and (3) can be written in the one-dimensional case as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0\,, \quad \frac{\partial \rho u}{\partial t} + \frac{\partial\,(p + \rho u^2 + \rho V^2)}{\partial x} = -f_w\,,$$

$$\frac{\partial \rho \left(e + e_v + u^2/2\right)}{\partial t} + \frac{\partial \rho u \left(h + e_v + u^2/2\right)}{\partial x} + \frac{\partial \rho u V^2}{\partial x} = -\frac{\partial Q_\tau}{\partial x}\,, \tag{10}$$

$$p = \rho e\,(\gamma - 1)\,, \quad p = \frac{R_0}{\mu}\rho T_g\,, \quad V^2 = 2e_v/3\,, \quad f_w = 4\tau_w/d\,,$$

$$\rho \frac{de_v}{dt} = J - \rho V^2 \frac{\partial u}{\partial x} - D_\tau\,. \tag{11}$$

Here $D_\tau = \overline{\tau'_{ij} s'_{ij}}$ and Q_τ are determined by relations (5) and (8). The overbar is omitted; all the variables are time- and cross section-average. It is noteworthy that the second term on the right-hand side of Eq. (11) describes a change (due to the medium's compressibility) in the energy of turbulent pulsations in the flow core. For subsonic velocities, this process can be disregarded compared to the generation in the boundary layer. Then the equation for the pulsation energy is simplified:

$$\rho \frac{de_v}{dt} = J - D_\tau . \tag{12}$$

To close system (10) and (12) we must determine J, l, and L (or Δ).

Hypothesis for the Generation of Pulsations in the Boundary Layer. The interior of the turbulent boundary layer consists of a laminar sublayer and a sublayer with a logarithmic velocity profile [5]. Pulsation energy is generated mainly in the logarithmic sublayer as a result of the restructuring of flow. It would appear natural that the "uncompensated heat" q'' of the unrealized laminar boundary layer, i.e., the layer that would be formed (in the case of its possible existence) instead of the turbulent one and would correspond to the averaged flow in the flow core, is converted to the pulsation energy. The logarithmic velocity profile is the residual profile after the transformation of part of the kinetic energy of the unrealized laminar boundary layer to the pulsation energy. The rate of generation of the "uncompensated heat" per unit volume is prescribed by the equality [4] $\rho dq''/dt = \tau_{ij} s_{ij}$. In the wall part of the laminar boundary layer, we have $\rho dq''/dt = \tau_{ij} s_{ij} \approx \tau_w \partial u/\partial y \approx \tau_w u_*/l_*$ [3]. Here $l_* = \nu_*/u_*$ and $u_* = \sqrt{\tau_w/\rho}$. Thus, the generation rate averaged over the channel cross section can be evaluated by the relation

$$J = \pi d \delta \tau_w u_* \Big/ \left(l_* \pi d^2/4 \right). \tag{13}$$

Dynamic length is the only dimension of length characteristic of the interior of the turbulent boundary layer. Therefore, the average size of the turbulent vortices formed in the boundary layer must be determined by the dynamic length l_*. On the other hand, the absence of turbulence in the laminar subregion is attributable to the fact that the size of vortices generated is of the order of the thickness of this sublayer δ_λ, i.e., $l \approx \delta_\lambda \approx 10 l_*$ [5]. Then the dissipation rate (5) can be evaluated from the formula

$$D_\tau = \overline{\tau'_{ij} s'_{ij}} \approx 0.20 \mu_* e_v / l_*^2 . \tag{14}$$

Steady-state turbulent flows in long smooth tubes with a diameter of 1 to 10 cm are experimentally investigated in [7]. The tube length-to-diameter ratio varies within 70–200; the values of the Reynolds numbers vary from $3 \cdot 10^3$ to $3 \cdot 10^6$. As a result of the processing of experimental data it has been established that the pulsation velocity V and the turbulence scale L under the conditions in question can be calculated from simple algebraic formulas [8]

$$V = 9 \cdot 10^{-2} u / \mathrm{Re}^{0.16}, \quad L = 0.1 d . \tag{15}$$

The distribution (obtained in the experiments) of velocity fluctuations across the flow shows that the velocity maximum is attained at a distance of $0.1d$ from the channel wall [7, 8]. Consequently, the turbulence scale and the thickness of the interior of the turbulent boundary layer can be evaluated by the relations

$$L \approx \Delta \approx 0.1 d , \quad \delta \approx 0.2 \Delta \approx 0.02 d . \tag{16}$$

In the turbulent flows investigated, pulsation energy along the tube remains constant in practice, i.e., $de_v/dt = 0$. In accordance with (12), this means that equilibrium is established between the generation and dissipation of pulsation energy in each cross section of the tube. The equality $J = D_\tau$ with account for expressions (13) and (14) takes the form

$$\frac{4 \delta \tau_w u_*}{l_* d} = \frac{0.2 \mu_* e_v}{l_*^2} . \tag{17}$$

In the case of slow flows we can evaluate τ_w, u_*, and l_* by the parameters of the averaged flow, using the relations for an incompressible fluid. In smooth tubes [3], we have $u_*^2 = u^2 (0.0032 + 0.221 \mathrm{Re}^{-0.237})/8$, where $\mathrm{Re} = ud/\nu_*$. With account for (16), equality (17) is reduced to the relation

$$W \approx 0.3 u \, (0.0032 + 0.221 \mathrm{Re}^{-0.237})^{1/2} . \tag{18}$$

Hence for $\mathrm{Re} << 25\cdot10^6$ the pulsation velocity is $V \approx 9\cdot10^{-2}u/\mathrm{Re}^{0.12}$, which is close to the first relation of (15). Thus, relations (15) can be interpreted as the conditions of equilibrium between the generation and dissipation of pulsation energy in steady-state turbulent flow in the tube. In this case they can be used instead of the differential equation (12) to close the one-dimensional equations (10).

Model of an Infinitely Thin Flame Front. In the present work, in studying the propagation of combustion of a gas in smooth tubes, we assume that turbulence develops between the flame and the head shock wave. For example, the structure of the gas flow ahead of the accelerating flame in experiments with a mixture of hydrogen and oxygen appears turbulent [9]. The length of the combustion zone δ_f is determined by the characteristic time of the chemical processes τ_c and the thermal diffusivity of the medium χ [1]: $\delta_f \approx \sqrt{\chi\tau_c}$. When it is believed that turbulence preserves the characteristic time of chemical reactions in order of magnitude, the thickness of the turbulent-combustion zone can be evaluated from the formula $\delta_\tau \approx \delta_n\sqrt{\chi_\tau/\chi_\lambda} \approx \delta_n\sqrt{\lambda_\tau/\lambda}$. If the quantity δ_τ is much smaller than the tube diameter, the combustion zone can be considered as the flame front. In methane-air mixtures, we have, e.g., $\delta_n \approx 0.5$ mm [10]. If the coefficients of turbulent and molecular thermal conductivities differ by two orders of magnitude ($\lambda_\tau \approx 10^2\lambda$), the thickness of the turbulent flame front is equal to about 0.5 cm in these mixtures. Therefore, it is hoped that the model of an infinitely thin flame front applies to tubes with a diameter of more than 5 cm. In the general case we must check the fulfillment of the inequality $\delta_\tau \approx \delta_n\sqrt{\lambda_\tau/\lambda} << d$.

Formulation of the Problem and Procedure of Solution. The processes of heat release and heat conduction beyond the flame front can be disregarded. Then (10) and (12) are reduced to equations close to the Euler equations for a relaxing gas in the form:

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho u}{\partial x}=0\,,\quad \frac{\partial\rho u}{\partial t}+\frac{\partial\,(p+\rho u^2+\rho V^2)}{\partial x}=-f_w\,,\quad \frac{\partial\rho\left(e+e_v+u^2/2\right)}{\partial t}+\frac{\partial\rho u\left(h+e_v+u^2/2\right)}{\partial x}+\frac{\partial\rho uV^2}{\partial x}=0\,,$$

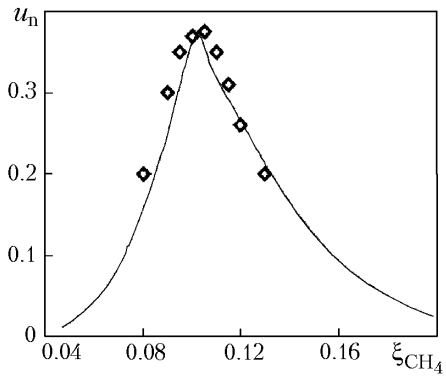
$$p=\rho e\,(\gamma-1)\,,\quad T_g=\frac{R_0}{\mu}\frac{p}{\rho}\,,\quad e_v=3V^2/2\,,\quad f_w=4\tau_w/d\,,\quad \rho de_v/dt=J-D_\tau\,. \tag{19}$$

Inhomogeneities of dimension $l \approx 1$ mm associated with turbulent vortices are observed in the flow in experiments on investigation of the turbulent combustion of methane-air mixtures [10]. But the average pulsation velocity V is five to ten times higher than the normal velocity of a laminar flame. Therefore, despite the comparability of the turbulent modes to the laminar-flame thickness ($\delta_n \approx 0.5$ mm) in size, the condition of realization of the so-called "volume combustion" is observed in these experiments [10]; in this combustion, the time of turbulent mixing is shorter than the time of the chemical processes $l/V < \delta_n/u_n$. The velocity of propagation of a turbulent flame u_τ relative to the averaged flow is calculated from the Damköhler–Shchelkin formula

$$u_\tau = u_n\sqrt{1+\lambda_\tau/\lambda}\,. \tag{20}$$

It is well known that the development of turbulent combustion may cause it to change to detonation easily realizable in the mixtures of gaseous hydrocarbons and oxygen. However there are no experiments that confirm the possibility of the detonation forming, e.g., in methane-air mixtures in smooth tubes in the case where reflected waves are weakly initiated or absent. In such "inert" gases, the initial acceleration of the flame results in combustion regimes with a limited velocity of propagation. In this connection, the regimes of turbulent combustion with a constant velocity of propagation are primarily of interest, since their existence guarantees, with a high degree of probability, the impossibility of combustion-to-detonation transition. In this case we must have the region of steady-state turbulent flow ahead of the zone of turbulent combustion. Therefore, in the problem considered below on the existence of the regimes of turbulent combustion with a constant velocity of propagation, we use either the first equation from (15) or the theoretical relation (18) close to it instead of the differential equation (12) for the "nonequilibrium" parameter e_v. The resulting regimes can arbitrarily be called "equilibrium" ones by analogy with relaxing-gas flow.

As the initial state of the medium we consider flow formed in propagation of the laminar flame front from the closed end in a semiinfinite tube [1]: the gas is quiescent behind the flame front; the flow in the region between the leading shock wave and the flame front is homogeneous. The intensity of the shock wave and its position at the



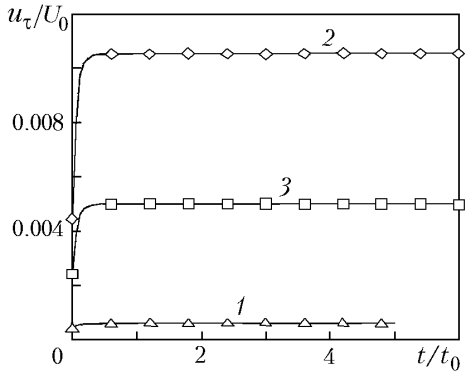


Fig. 1. Normal velocity of the laminar flame in methane-air mixtures: points, experiment, curve, computation.

Fig. 2. Formation of the "equilibrium" velocity of propagation of a turbulent flame in methane-air mixtures: 1) 7%, 2) 11%, and 3) 13% methane.

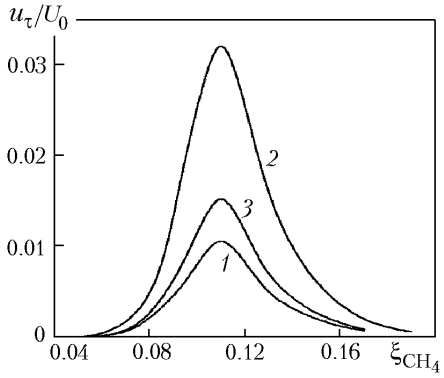
initial instant of time are determined by the normal velocity of the flame front u_n and its distance from the end wall. If the Reynolds number between the leading shock wave and the flame front is Re > 1000, the turbulence of the flow is taken into account. The flame velocity u_τ corresponding to this state of the medium is calculated from formula (20) with the use of relations (8) and (15) for the turbulent thermal conductivity and the pulsation velocity. From the value of the flame velocity, computed in such a manner, and Eqs. (19), we determine a new distribution of the flow parameters. Next, we calculate again the turbulent-flame velocity corresponding to the new pulsation characteristics of the flow behind the leading shock wave, etc. The regime with a constant velocity of propagation of combustion can be formed after a certain number of such time iterations.

The problem is solved numerically by the S. K. Godunov method [11] with the use of a moving computational grid. One grid node is brought into coincidence with the frame front, whereas the last mode is made to agree with the head shock wave. The total velocity of propagation of the flame is determined by solution of the problem on disintegration of an arbitrary discontinuity in a fuel gas [12] using expression (20) for the relative velocity of a turbulent flame u_τ. The normal velocity of propagation of a laminar flame u_n is determined by the composition of the mixture and is calculated according to the procedure of [13]; the turbulent-thermal-conductivity coefficient λ_τ is computed from formula (8), and the molecular-thermal-conductivity coefficient of the mixture λ is calculated from the Wilke formula [14]. The necessary parameters of the averaged flow are taken in the cell just ahead of the flame front.

Results of Calculations for Methane and Hydrogen-Air Mixtures in Semiinfinite Smooth Tubes. The calculated values of the normal velocity of propagation of a laminar flame in methane-air mixtures (Fig. 1) are in good agreement with the data of experiments [8]. To reveal the distinctive features of the propagation of turbulent combustion we disregard friction in the first step. In the figures below, the distances are given in meters; velocity and time are referred to the quantities $U_0 = \sqrt{p_0/\rho_0}$ and $t_0 = l_0/U_0$. Here l_0 = 1 m and d = 0.1 m.

The dynamics of change in the relative velocity u_τ for three methane-air mixtures is presented in Fig. 2. First u_τ grows but its value is stabilized with time, which means the formation of an equilibrium regime of turbulent combustion with a constant velocity of propagation. It is noteworthy that change in the flame velocity (see Fig. 2) does not describe the actual process, since the equilibrium relation (15) is used for pulsation energy instead of the differential equation.

Figure 3 plots the "equilibrium" velocity as a function of the content of methane for d = 0.1 m (curve 1) and d = 0.5 m (curve 2). The velocity of propagation of the turbulent combustion of a 11% methane-air mixture in a tube of diameter 0.1 m is equal to nearly 3 m/sec. Curve 3 for d = 0.1 m has been obtained with the use of the theoretical dependence (18) for the pulsation-velocity modulus W instead of the experimental relation (15). The difference between the "experimental" curve 1 and the "theoretical" one 3 is no higher than 30%. The values of the Reynolds numbers in the turbulent flow just ahead of the combustion front of different methane-air mixtures are presented in Fig. 4 by the



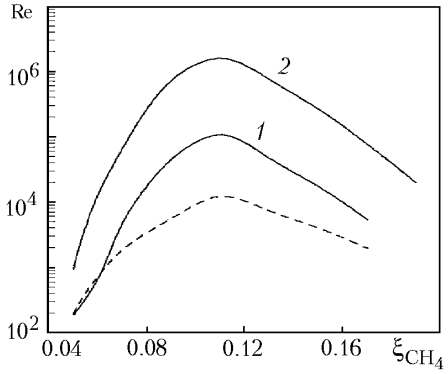
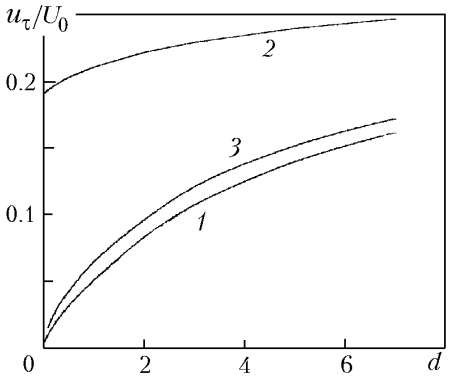


Fig. 3. "Equilibrium" velocity of propagation of the turbulent combustion of methane-air mixtures: 1 and 2) obtained with the use of the experimental relations (15); 3) from relation (18).

Fig. 4. Reynolds number in the flow ahead of the flame front vs. molar concentration of methane in the mixture: 1) d = 0.1 and 2) 0.5 m; dashed curve, for the laminar flow in the tube with d = 0.1 m.



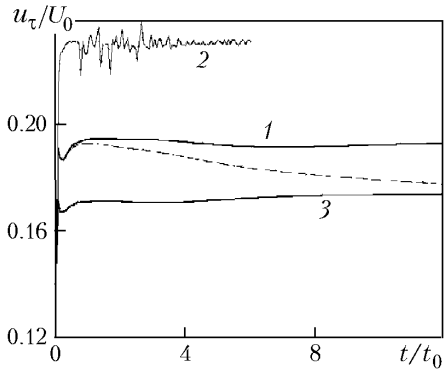


Fig. 5. Velocity of propagation of the turbulent combustion of a 11% methane-air mixture vs. channel diameter: 1) calculation from relations (15); 2) flame velocity in the Chapman–Jouguet regime; 3) calculation from relation (18).

Fig. 6. Formation of the "equilibrium" velocity of propagation of the turbulent combustion of methane-oxygen mixtures for d = 0.1 m: 1) 18, 2) 22, and 3) 45% methane; dashed curve, with allowance for friction with 18% methane.

solid curves. A logarithmic scale with a base of 10 is used along the ordinate axis. The dashed curve corresponds to the Reynolds numbers in the flow ahead of the laminar flame front in the case where d = 0.1 m.

The results obtained are in agreement with the data of the experiments conducted by Damköhler, Williams, and Bollinger for mixtures of air and other gaseous hydrocarbons [8] as far as the order of magnitude and the qualitative dependence on the composition and the Reynolds number are concerned.

The velocity grows with overall dimensions of the tube and the concentration limits of turbulent combustion become wider. It is assumed that, in tubes of a fairly large diameter, the flame velocity u_τ reaches the values of the Chapman–Jouguet velocity on the lower branch of the adiabat with heat release.

A nearly stoichiometric mixture with 11% methane seems the most promising for this purpose. Calculations show that the "equilibrium" flame velocity grows indeed (Fig. 5, curve 1), but does not reach the Chapman–Jouguet velocity (curve 2) characteristic of the flow formed ahead of the flame front. Curve 3 refers to the turbulent-flame ve-

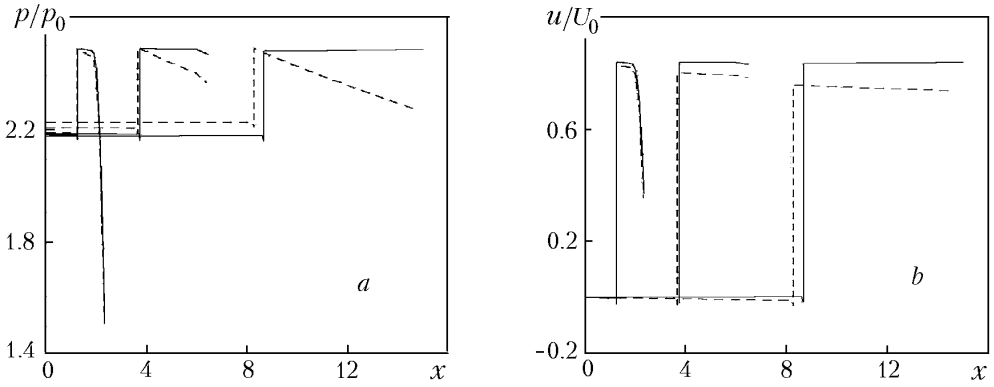


Fig. 7. Distribution of the pressure (a) and the velocity (b) of the gas in a 18% methane-oxygen mixture.

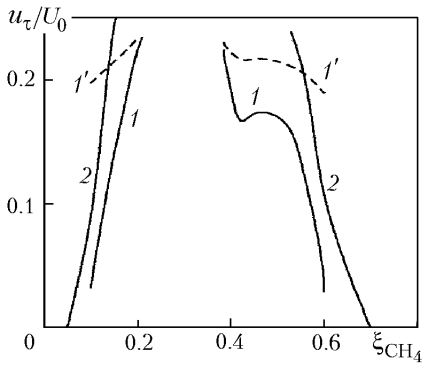
locity calculated with the use of relation (18) for the pulsation velocity. Excess over the Chapman–Jouguet velocity means that the preparation of the mixture for ignition as a result of the transfer of heat from the heat-release zone is shorter than the period over which the gas can burn in the deflagration regime. In this case conditions for the explosive release of energy in the heated gas volume and for the explosive transformation of the flame front to a detonation wave are formed just ahead of the combustion front, which is observed in experiments [10, 15] with oxygen mixtures.

Thus, the above calculation results show that no combustion-to-detonation transition is realized in semiinfinite smooth tubes filled with methane-air mixtures. In experiments with the mixtures of gaseous hydrocarbons and air, this process is carried out only in the presence of reflected shock waves.

Mixtures of methane and oxygen are characterized by the higher heat release, the higher velocity of propagation, and consequently the higher-than-average level of turbulization. However, if the content of methane does not exceed 20% or is higher than 40%, the regime of turbulent combustion with a constant rate (which is no higher than the Chapman–Jouguet velocity, just as in methane-air mixtures) is being smoothly reached in a tube with a diameter d = 0.1 m. The dynamics of formation of the rate of turbulent combustion in the mixtures of 18% and 45% methane and oxygen is presented in Fig. 6 by curves 1 and 3. The numerical solution becomes self-similar with a constant velocity of propagation of the flame and the head shock with time; this self-similar solution is allowed by Eqs. (19) in the absence of friction. The turbulent flame front separates the combustion products from the unburned gas. Constant values of the gasdynamic parameters of the flow are established in each flow region (solid curves in Fig. 7). In the laminar case the intensity of the head shock wave is low in these mixtures. Thus, for 18% methane, the Mach number of the wave is M_h = 1.033, the pressure is $p = 1.077p_0$, and the gas temperature is $T_g \approx 300$ K at a temperature of the unperturbed medium of 293 K. Ahead of the turbulent flame front, in this mixture of methane and oxygen, we have $p = 2.5p_0$ and $T_g \approx 390$ K; the Mach number of the head shock wave is M_h = 1.5. However, the intensity of the head shock wave turns out to be insufficient for the ignition of the gas just behind it. This is consistent with experimental observations: detonation continues uninterruptedly, in practice, the propagation of the deflagration front even in a stoichiometric mixture of hydrogen and oxygen [10, 15].

In mixtures with a concentration of methane lower than 20% and higher than 40%, the relative velocity of the turbulent flame (Fig. 8), curve 1) is smaller than the Chapman–Jouguet velocity (curve 1′). Within this concentration interval, the turbulent-flame velocity formally computed from formula (20) exceeds the Chapman–Jouguet velocity, which is inconsistent with the laws of gas dynamics. In the calculations, the turbulent-flame velocity is bounded, which makes it possible to formally continue computations. As a result, e.g., in the mixture with 22% methane, the flame velocity does not reach a constant value and begins to pulsate randomly when the Chapman–Jouguet velocity is attained (Fig. 6, curve 2).

The same concentration interval is observed in hydrogen-air mixtures. In Fig. 9, the solid curves refer to the velocity of turbulent combustion in tubes of different size as a function of the molar concentration of hydrogen. The velocities of the combustion wave in the Chapman–Jouguet regime for the parameters in the flow ahead of the combustion front in a tube of diameter 0.5 m are shown by the dashed curves. The limits of the interval under study become wider with increase in the channel diameter.



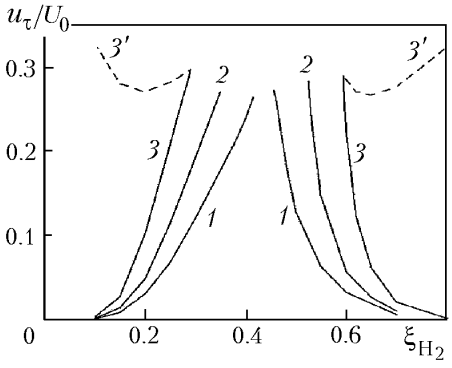


Fig. 8. "Equilibrium" rate of turbulent combustion vs. molar concentration of methane in mixtures with oxygen: 1) d = 0.1 and 2) 0.5 m; 1′) flame velocity in the Chapman–Jouguet regime for d = 0.1 m.

Fig. 9. "Equilibrium" rate of turbulent combustion vs. molar concentration of hydrogen in mixtures with air: 1) d = 0.1, 2) 0.2, and 3) 0.5 m; 3′) flame velocity in the Chapman–Jouguet regime for d = 0.5 m.

Thus, in methane-oxygen and hydrogen-air mixtures, we have a concentration range in which there are no "equilibrium" regimes of turbulent combustion with a constant velocity of propagation, which points to the possibility of deflagration-to-detonation transition in smooth tubes of a fairly large diameter.

The concentration limits obtained for the transition of the combustion of methane with oxygen to detonation are in agreement with experimental data [16].

Friction on the channel walls scarcely affects the velocity of propagation of the turbulent combustion of methane-air mixtures because of the low velocity of gas flows. The corresponding curve is coincident, in practice, with curve 1 in Fig. 5. In the mixtures of methane and oxygen, friction diminishes the velocity of propagation of combustion (Fig. 6, the dashed curve). The gasdynamic parameters behind the head shock wave do not maintain a constant value (dashed curves in Fig. 7).

CONCLUSIONS

1. The hypotheses proposed for the generation and dissipation of pulsation energy lead to results that are in satisfactory qualitative and quantitative agreement with the data of experiments on the average pulsation velocity in propagation of turbulent combustion in smooth tubes.

2. In semiinfinite smooth tubes, the combustion of methane-oxygen mixtures propagates with a velocity not exceeding the Chapman–Jouguet velocity on the lower adiabatic branch with heat release which is characteristic of the averaged flow formed ahead of the flame front. The flame velocity grows with tube diameter, and the concentration limits of existence of turbulent combustion regimes become wider. However, the ignition of methane with air does not lead to a detonation combustion of the mixture.

3. Combustion-to-detonation transition is possible as a result of the explosive release of energy ahead of the turbulent flame front, when the removal of heat together with combustion products from this region by convective flows becomes smaller than the heat inflow due to turbulent heat conduction.

4. In methane-oxygen and hydrogen-air mixtures, we have a detonationally hazardous range of fuel concentrations (localized near the stoichiometric composition), in which deflagration-to-detonation transition is possible in smooth tubes of a fairly large diameter.

5. Friction on the walls does not affect, in practice, the velocity of propagation of the turbulent combustion of methane-air mixtures in smooth tubes but becomes appreciable in mixtures of methane and oxygen.

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NOTATION

$\overline{A}_\mu$, work of viscous stresses; $\overline{A}_\tau$, work of Reynolds stresses; A'_τ, work due to viscous-stress pulsations; c_p, specific heat at constant pressure; C_*, coefficient of resistance to the motion of turbulent vortices; d, tube diameter, m; D_τ, rate of dissipation of pulsation energy; e, thermal energy of the gas; e_v, average energy of velocity pulsations; $\mathbf{f}$, vector of the force inhibiting the propagation of pulsations in the average flow; f_w, friction force on the channel walls; h, enthalpy of the gas; I_{ij}, correlation coefficient of the ith and jth components of the unit vector of pulsation velocity; J, intensity of generation of pulsations in the turbulent boundary layer; l, average size of a vortex; l_0, characteristic length, m; l_*, dynamic length in the turbulent boundary layer; L_*, full turbulence scale; L, turbulence scale along one Cartesian coordinate; M_h, Mach number of the head wave; n, concentration of turbulent vortices per unit volume; p, pressure; p_0, pressure of an unperturbed gas; p_1, pressure of the "basic" phase; p_2, pressure of the "fictitious" phase; q'', "uncompensated heat" of the laminar boundary layer; $\overline{Q}_{\lambda j}$ and $\overline{Q}_{\tau j}$, components of the molecular and turbulent heat fluxes; $\mathbf{r}$, radius vector of a spatial point; r, modulus of the vector $\mathbf{r}$; R_0, universal gas constant; Re, Reynolds number computed from the molecular viscosity and the average velocity of the flow in the tube; Re_*, Reynolds number of the pulsation motion of turbulent vortices; $\overline{R}_{ij}$, Reynolds-stress tensor; S, cross-sectional area of one turbulent vortex; s_{ij}, strain-rate tensor; t, time, sec; t_0, characteristic time, sec; T_g, gas temperature; T, averaging period; u, average flow velocity along the tube axis, m/sec; u_n, normal velocity of propagation of the laminar flame, m/sec; u_τ, velocity of propagation of the turbulent flame relative to the gas ahead of it, m/sec; u_*, dynamic velocity in the turbulent boundary layer; U_0, characteristic velocity, m/sec; $\mathbf{u}$, velocity vector; $\mathbf{u}'_{un}$, unit vector of pulsation velocity; V, averaged value of the pulsation-velocity modulus in one direction; W, averaged value of the pulsation-velocity modulus; x, distance from the end tube wall, m; x_j, Cartesian coordinates of the vector $\mathbf{r}$; α, longitude of the end of the unit vector of pulsation velocity in the Cartesian coordinate system; γ, ratio of the specific heats of the gas; δ and δ_λ, thickness of the anisotropic part and the laminar subregion of the turbulent boundary layer; δ_f, length of the combustion zone; δ_n and δ_τ, thickness of the zone of laminar (normal) and turbulent combustion; δ_{ij}, Kronecker symbol; Δ, thickness of the turbulent boundary layer; $\Delta\mathbf{r}$, increment in the vector $\mathbf{r}$; θ, latitude of the end of the unit vector of pulsation velocity in the Cartesian coordinate system; λ, molecular-thermal-conductivity coefficient; λ_τ, turbulent-thermal-conductivity coefficient under local-isotropy conditions; λ_{ij}, tensor of turbulent-thermal-conductivity coefficients; μ_*, coefficient of molecular viscosity; ν_*, kinematic coefficient of viscosity; ξ_{CH_4} and ξ_{H_2}, molar fraction of methane and hydrogen in the starting mixture; ρ, density of the gas; ρ_0, density of an unperturbed gas; τ_w, friction stress on the channel wall; τ_c, characteristic time of the chemical processes; τ_{ij}, viscous-stress tensor; φ_j, angles of inclination of the pulsation-velocity vector to the axes of the Cartesian coordinate system; χ, thermal diffusivity of the gas; χ_λ and χ_τ, thermal-diffusivity coefficients in the laminar and turbulent flow; Ψ, arbitrary quantity; Ψ, time-averaged arbitrary quantity; Ψ', pulsation of the arbitrary quantity; $d\Omega$, area of the surface element of a unit sphere. Subscripts: c, chemical; CH_4, methane; un, unit; f, flame; g, gas; h, head; H_2, hydrogen; i and j = 1, 2, and 3 according to the number of coordinate axes; n, normal; v, vibrational; w, on the channel wall; λ, laminar; μ, viscous; τ, turbulent; 0, initial or standard parameter; 1 and 2, first and second phases; *, presence of friction; ′, pulsations of the corresponding quantities.

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