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CRITICAL DIAMETERS OF POROUS MEDIUM PARTICLES IN NON-ADIABETIC FILTRATION COMBUSTION OF METHANE-AIR MIXTURE

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Abstract. This paper examines the velocity and equilibrium temperature of a stationary wave of filtration combustion of gases as a function of the fuel-equivalent ratio. Calculations of the stationary wave velocity and equilibrium temperature were performed using previously obtained relationships. The calculations revealed that positive values ??of the hydrogen-air mixture wave velocity, and consequently, superadiabatic equilibrium temperatures, occur only for sufficiently saturated or extremely fuel-lean mixtures. During combustion of a methane-air mixture, both copropagation and counterpropagation of the combustion wave occur. The equilibrium temperature of the methane-air mixture is higher than that of hydrogen-air and propane-air mixtures, and the superadiabatic temperature is achieved in the fuel-rich region, at less saturated mixture compositions. The stationary wave of filtration combustion of a propane-air mixture predominantly propagates in a counterpropagation direction and exhibits subadiabatic equilibrium combustion temperatures.

1. Introduction

Introduction. During gas combustion, the balance of air and combustible gas plays a crucial role. When these two primary combustion components are in balance, that is, during a stoichiometric reaction, the maximum flame temperature, maximum reaction rate, and greatest chemical activity are achieved. However, combustion does not always occur with a stoichiometric ratio of components. Most often, an imbalance occurs, leading to a decrease in combustion temperature, flame instability, the formation of harmful combustion products (during hydrocarbon combustion), and, ultimately, a decrease in the combustion efficiency of combustible gases. Therefore, when studying gas combustion, it is important to consider cases of fuel deficiency or excess [1-4].

Typically, studies of gas combustion, including filtration combustion, taking into account the fuel-to-fuel ratio are conducted experimentally [5-8]. While experimental studies provide a relatively accurate understanding of the process, they have limited ability to vary the parameters that influence combustion characteristics.

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This shortcoming of experimental studies is particularly noticeable in filtration combustion, as this type of combustion is characterized by its multiparameter nature. Therefore, it is necessary to develop a theoretical approach to studying the influence of the fuel-to-fuel ratio on the characteristics of the filtration combustion wave. The developed theoretical approach would allow for studies to be conducted over the widest possible range of parameters influencing filtration combustion, enabling a more detailed study of the combustion process. Therefore, the search for the development of such a theoretical approach is highly relevant.
This paper proposes a theoretical approach to studying the effect of the fuel-to-fuel ratio on the velocity and temperature of the steady-state combustion wave of gases. Based on this approach, we calculate the wave velocity and equilibrium temperature with varying fresh mixture injection rates. Hydrogen, methane, and propane-air mixtures are considered.

2. Mathematical model

In the work [9] a single-temperature stationary mathematical model of filtration combustion of gases was considered, recorded in a moving at a constant speed U coordinate system [10, 11]

$$\begin{gathered}(\rho_{10}c_p(\upsilon_{10}-U)+\rho_2c_2U)\frac{dT}{dx}=\frac{d}{dx}((\alpha_1\lambda_1+\alpha_2\lambda_2)\frac{dT}{dx})+\rho_1QJ,\\ (\rho_{10}(\upsilon_{10}-U))\frac{d\eta_{1(i)}}{dx}=\frac{d}{dx}((\rho_1D_{(i)})\frac{d\eta_{1(i)}}{dx})+\rho_1\zeta_{1(i)}J,\ \ i=1,2,3,...,k,\\ J=\eta_{1(k_*)}k_0exp(-E/(RT)),\ \ \rho_1T_1=\rho_{10}T_0,\\ \zeta_{1(i)}=-\frac{g_{1(i)}(\nu''_{1(i)}-\nu'_{1(i)})}{g_{1(k_*)}(\nu''_{1(k_*)}-\nu'_{1(k_*)})},\end{gathered}\tag{2.1}$$

with boundary conditions

$$\begin{gathered}x=-\infty:,\ T=T_0,,\ \ \eta_{1(i)}=\eta_{1(i)0},,\ \ \frac{dT}{dx}=0,,\ \ \frac{d\eta_{1(i)}}{dx}=0,\\ x=+\infty:,\ T=T_e,,\ \ \eta_{1(i)}=\eta_{1(i)e},,\ \ \frac{dT}{dx}=0,,\ \ \frac{d\eta_{1(i)}}{dx}=0,\end{gathered}\tag{2.2}$$

Here T, — ambient temperature; $\eta_{1(i)}$ — mass concentration of the i-th component of the gas mixture; $\eta_{1(k_*)}$ — mass concentration of the missing component; υ_{10} — gas flow rate in pores; ρ_{10}, c_p — the reduced density and heat capacity of the gas mixture, respectively; ρ_2, c_2 — the same values for a porous medium; λ_1, λ_2 — thermal conductivity coefficients of gas and porous medium; α_1, α_2 — volumetric contents of gas and porous medium; Q — thermal effect of a chemical reaction; J — the rate of a chemical reaction; E — activation energy; R — universal gas constant; k_0 — pre-exponent; $\nu'_{1(i)}, \nu''_{1(i)}$ — stoichiometric coefficients of the initial and final substances, respectively; $g_{1(i)}$ — molecular weights of the components of the gas mixture; T_0 — ambient temperature; ρ_1 — mixture density; $D_{1(i)}$ — diffusion coefficient of the i-th component of the gas mixture.

As a result of the study of system (1), a relation was obtained for the velocity of a stationary combustion wave

$$(\upsilon_{10}-U)^2=\frac{k_0\exp(-1/\beta)\alpha_1\gamma\lambda_1\Lambda T_0}{\rho_{10}c_pu_\varphi\eta_{1(k_*)0}T_e}\times$$
$$\times(\eta_{1(k_*)0}+\frac{\eta_{1(k_*)e}-\eta_{1(k_*)0}}{1+A_{(k_*)}}+(\eta_{1(k_*)e}-\eta_{1(k_*)0})\sum_{i=1}^{k}\frac{\eta_{1(i)e}-\eta_{1(i)0}}{1+A_{(2)}+A_{(i)}}+ \tag{2.3}$$
$$+\eta_{1(k_*)0}\sum_{i=1}^{k}\frac{\eta_{1(i)e}-\eta_{1(i)0}}{1+A_{(i)}}),$$

where

$$A_{(i)}=\frac{\gamma}{Le_{eff(i)}u_\varphi},\ \ Le_{eff(i)}=\frac{Le_i}{\Lambda},\ \ \Lambda=1+\frac{\alpha_2\lambda_2}{\alpha_1\lambda_1},\ \ Le_i=\frac{D_{1(i)}\rho_{10}c_p}{\alpha_1\lambda_1},$$

$$u_\varphi=1-\frac{\varphi}{u_0-1},\quad \varphi=\frac{\rho_2c_2}{\rho_{10}c_p},\quad u_0=\frac{\upsilon_{10}}{U},\ \ \beta=\frac{RT_e}{E},\ \ \gamma=\frac{RT_e^2}{E(T_e-T_0)},$$

$$T_e=\frac{Q(\eta_{1(k_*)0}-\eta_{1(k_*)e})}{c_pu_\varphi}.$$

This study assumes that thermal conductivity and convective heat transfer make the primary contributions to combustion wave propagation in a porous block, while the influence of diffusion processes is considered insignificant. In this case, from relation (2), as the diffusion coefficients of the components tend to zero, i.e., if these coefficients are neglected, one can obtain a relation for the combustion wave velocity

$$(\upsilon_{10}-U)^2=\frac{k_0\exp(-1/\beta)\alpha_1\gamma\lambda_1\Lambda T_0}{\rho_{10}c_pu_\varphi T_e}. \tag{2.4}$$

A theoretical approach to studying the influence of the fuel-fuel ratio. As a rule, the fuel-fuel ratio is determined relative to the stoichiometric mixture using the formula [5]

$$\phi=\frac{\eta_f}{1-\eta_f}:\frac{\eta_{f,cm}}{1-\eta_{f,cm}}. \tag{2.5}$$

Here η_f, $\eta_{f,cm}$ — concentration and stoichiometric concentration of combustible gas in the gas-air mixture, $1-\eta_f$, $1-\eta_{f,cm}$ — concentration and stoichiometric concentration of air in the gas-air mixture. At $\phi<1$ the mixture is considered lean in fuel, and when $\phi>1$ — rich. The stoichiometric mixture corresponds to the case $\phi=1$. Meaning $\eta_{f,cm}$ is determined from the stoichiometric equation, and η_f determined at a given value ϕ.

The equilibrium temperature of the medium (gas mixture + porous medium) is determined by the formula

$$T_e = \frac{Q(\eta_{1(k_*)0} - \eta_{1(k_*)e})}{c_p u_\varphi}. \tag{2.6}$$

In formula (2.6) $\eta_{1(k_*)0}$ — initial concentration of the reacting component, $\eta_{1(k_*)e}$ the remainder of the reacting component, $\eta_{1(k_*)0} - \eta_{1(k_*)e}$ — the amount of the reacting component entering into the reaction. When burning a hydrogen-air mixture, we'll assume that oxygen is the reactant. Therefore, to determine the equilibrium combustion temperature of a hydrogen-air mixture, it's necessary to find the amount of oxygen involved in the chemical reaction. In a fuel-rich region ($\phi > 1$) there is a shortage of oxygen, so all of it will be spent in a chemical reaction $\eta_{1(k_*)e} = 0$. Hence, in formula (2.6) the initial concentration of hydrogen is taken into account ($\eta_{1(k_*)0} = (1 - \eta_f) \cdot 0.21$). In a fuel-poor region ($\phi < 1$) the amount of oxygen for the reaction is excessive, therefore it is necessary to determine the amount of oxygen entering into the chemical reaction. It is assumed that (this assumption is confirmed by calculations) $\phi < 1$ the amount of oxygen entering into the reaction is proportional to the stoichiometric oxygen consumption, that is

$$1 - \eta_f = \frac{1 - \eta_{f,cm}}{\eta_{f,cm}} \eta_f.$$

From here at $\phi < 1$ in formula (2.6) is taken

$$\eta_{1(k_*)0} - \eta_{1(k_*)e} = \frac{1 - \eta_{f,cm}}{\eta_{f,cm}} \eta_f.$$

In the case of filtration combustion of methane and propane-air mixtures, the combustible gas will be considered the reactant component. Therefore, the combustion of methane and propane-air mixtures is considered in reverse order.At $\phi < 1$ there is a shortage of combustible gas, so it will be completely used up. Thus, the remainder is zero ($\eta_{1(k_*)e} = 0$) and in formula (2.6) we take into account that $\eta_{1(k_*)0} = \eta_f$. In a fuel-rich area ($\phi > 1$), it is also assumed that the consumption of combustible gas is comparable to the consumption of combustible gas in a stoichiometric mixture, and is determined as follows $\eta_{f,cm} - (\eta_f - \eta_{f,cm})$. Thus, when $\phi > 1$ formula (2.6) takes into account

$$\eta_{1(k_*)0} - \eta_{1(k_*)e} = \eta_{f,cm} - (\eta_f - \eta_{f,cm}).$$

When studying the combustion process of gases in air depending on the fuel excess ratio, it is important to take into account changes in the thermophysical properties of the mixture, namely, density, thermal conductivity, and heat capacity, since these characteristics of the mixture change with a change in the concentration of combustible gas in the mixture. In this work, the density, thermal conductivity, and heat capacity of the mixture depending on the fuel excess ratio are calculated using the following approximate formulas [12], respectively

$$\rho_s = \frac{1+(1/\phi)L_0}{1/\rho_f + 1/\rho_a}, \quad \lambda_s = \frac{\lambda_f + (1/\phi)L_0\lambda_a}{1+(1/\phi)L_0}, \quad c_{p,s} = \frac{c_{p,f} + (1/\phi)L_0 c_{p,a}}{1+(1/\phi)L_0}$$

where ρ_f, λ_f, $c_{p,f}$ — density, thermal conductivity and heat capacity of the combustible gas, respectively, ρ_a, λ_a, $c_{p,a}$ — density, thermal conductivity and heat capacity of air, respectively, L_0 - stoichiometric air consumption per kg of combustible gas.

The thermal effect of the reaction for each mixture was determined based on the stoichiometric coefficients and heat generation of the components of the chemical reaction, according to the formula:

$$Q = \Sigma_{k=1}^{n} \nu''_{1(k)} i_k - \Sigma_{k=1}^{m} \nu'_{1(k)} j_k,$$

where i_k and j_k — heat generation of the final and initial products of a chemical reaction, respectively.

3. Results and their discussion

Calculation results and discussion. The wave velocity and equilibrium temperature of hydrogen-, methane-, and propane-air mixtures were determined, respectively, by relations (4) and (6). The excess fuel coefficient for the hydrogen-air mixture was set from 0.1 to 6, with a step of 0.1, which corresponds to a hydrogen concentration in the mixture from 4 % to 72 %. For methane and propane, the coefficient varied from 0.4 to 2.2 and from 0.4 to 2, also with a step of 0.1, respectively, while their concentrations changed from 4 % to 19 % for methane and from 2 % to 8 % for propane. Note that in Fig. 1-3, negative values of the wave velocity correspond to counter-propagation relative to the flow of the freshly injected mixture, and positive values correspond to co-propagation.

The reliability of the obtained results is confirmed by the fact that the obtained results in the form of dependence curves have the same tendency with the experimental data, and the same orders of wave speed as in the experiment [6].

The calculations were carried out using the following values of the physical and chemical parameters of the porous medium and gas mixture [13]:

$$\text{1)hydrogen}: \ \alpha_1 = 0.5, \ \alpha_2 = 0.5, \ \rho_{10}^0 = 0.04 \ kg/m^3, \ \rho_{20}^0 = 3000 \ kg/m^3,$$
$$c_p = 14200 \ J/(kgK), \ c_2 = 660 \ J/(kgK), \ T_0 = 320, \ \lambda_1 = 0.168 \ W/(m^2K),$$
$$\lambda_2 = 0.2 \ W/(m^2K), \ E = 126000 \ J, \ Q = 2.68 \cdot 10^7 \ J, \ k_0 = 5 \cdot 10^{10} \ s^{-1},$$
$$R = 8.314 \ J/(molK).$$
$$\text{2)methane}: \ \alpha_1 = 0.5, \ \alpha_2 = 0.5, \ \rho_{10}^0 = 0.641 \ kg/m^3, \ \rho_{20}^0 = 3200 \ kg/m^3,$$
$$c_p = 2180 \ J/(kgK), \ c_2 = 800 \ J/(kgK), \ T_0 = 320, \ \lambda_1 = 0.031 \ W/(m^2K),$$
$$\lambda_2 = 4 \ W/(m^2K), \ E = 226000 \ J, \ Q = 3.107 \cdot 10^7 \ J, \ k_0 = 10^{11} \ s^{-1},$$
$$R = 8.314 \ J/(molK).$$
$$\text{3)propane}: \ \alpha_1 = 0.5, \ \alpha_2 = 0.5, \ \rho_{10}^0 = 1.764 \ kg/m^3, \ \rho_{20}^0 = 3200 \ kg/m^3,$$
$$c_p = 1570 \ J/(kgK), \ c_2 = 800 \ J/(kgK), \ T_0 = 320, \ \lambda_1 = 0.015 \ W/(m^2K),$$
$$\lambda_2 = 4 \ W/(m^2K), \ E = 131000 \ J, \ Q = 7.807 \cdot 10^7 \ J, \ k_0 = 5.4 \cdot 10^{13} \ s^{-1},$$

$$R = 8.314\ J/(molK).$$

$$4)air:\ \rho_a^0 = 1.163\ kg/m^3,\ c_{p,a} = 1006\ J/(kgK),\ \lambda_a = 0.025\ W/(m^2K).$$

As can be seen from Fig. 1a for low injection speeds (from 0.1 to 0.5 m/s) for all values ϕ the velocity of the hydrogen-air mixture wave is negative, which corresponds to the counter-movement of the combustion wave. Increasing the injection speed from 0.5 to 1.45 m/s increases the counter-movement velocity by an order of magnitude 10^{-3} m/s, and a further increase in the injection speed (6 m/s) showed that the wave speed does not exceed this order. Moreover, an increase in the injection speed from 0.5 to 6 m/s contributes to the emergence of regions ϕ, where co-movements of the combustion wave are possible. However, it should be noted that these positive regions of wave velocity values appear only when $\phi > 1$. In a fuel-poor region, with the injection speed varying from 0.1 to 6 m/s, co-current motion occurs only at the lower concentration limit of hydrogen ignition, that is, at $\phi = 0.1$, which corresponds 4% percent of hydrogen in the mixture. The change in the equilibrium temperature of the combustion wave of the hydrogen-air mixture is shown in Fig. 1b. Negative values of the wave velocity correspond to subadiabatic values of the equilibrium temperature. Since for low injection speeds (from 0.1 to 0.5 m/s) and for all values ϕ if only negative wave velocities occur, then subadiabatic equilibrium temperatures are achieved. Superadiabatic temperatures can be achieved by increasing the injection rate, but only with sufficiently rich or extremely lean fuel mixtures.

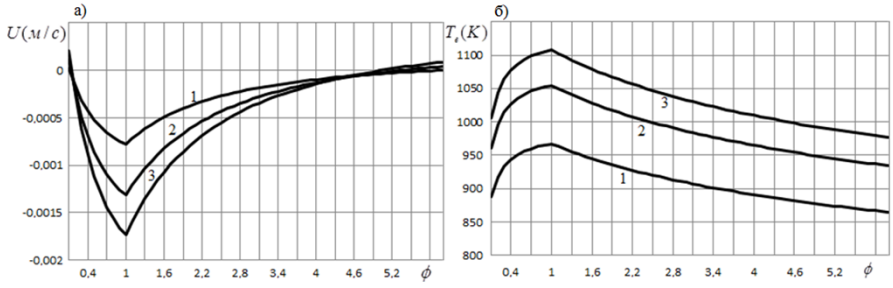

Figure 1. Curves of the dependence of the wave velocity (a) and the equilibrium temperature (b) of the hydrogen-air mixture on the excess fuel coefficient with varying mixture injection speed: $1 - - - 0.5, 2 - - - 1, 3 - - - 1.45 m/s$.

Looking at the curves of the methane-air mixture wave velocity (Fig. 2a), it can be seen that within the range of variation of the fuel excess ratio, both co-propagation of the combustion wave and counter-propagation of the combustion wave occur. Co-propagation of the combustion wave occurs predominantly at $\phi > 1$. In the fuel-poor region, as in the case of a hydrogen-air mixture, positive values ??of the wave velocity occur at relatively high injection rates and the lower concentration limit of methane, that is, $\phi = 0.4$, which corresponds 4% methane in the mixture. Note that, compared to the hydrogen-air mixture, co-propagation for the methane-air mixture takes place starting from $\phi > 1.6$, and for a hydrogen-air

mixture — $\phi > 4.7$, which is closer to stoichiometry for methane than for hydrogen. Here, the wave velocity is an order of magnitude lower than for a hydrogen-air mixture. Furthermore, the equilibrium temperature of a methane-air mixture is higher than for a hydrogen-air mixture, and the superadiabatic temperature is realized in the fuel-rich region, at less saturated mixture compositions, that is, starting from $\phi > 1.6$ (Fig. 2b). For comparison, with a hydrogen-air mixture, superadiabatic temperatures are realized in sufficiently fuel-saturated compositions, that is, starting from $\phi > 4.7$.

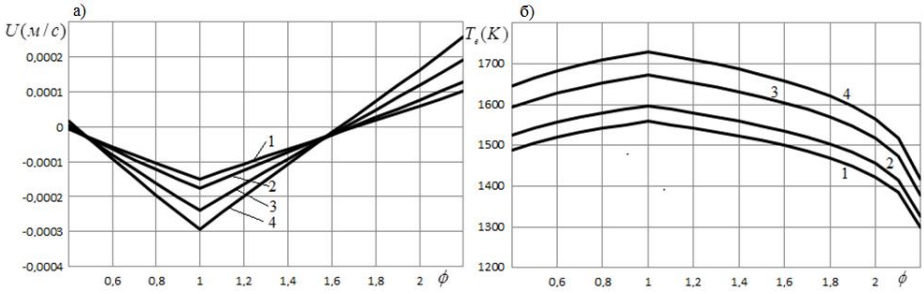

Figure 2.Curves of the dependence of the wave velocity (a) and the equilibrium temperature (b) of the methane-air mixture on the excess fuel coefficient with varying mixture injection speed: 1 — 0.24, 2 — 0.3, 3 — 0.45, 4 — 0.6 m/s.

The velocity of the combustion wave of the propane-air mixture in the range of change ϕ is negative, with the exception of the extreme point on the right, which corresponds to a concentration close to the upper flammability limit (Fig. 3,a). This trend is observed both for low injection speeds (0.1 m/s) and for relatively high ones (2 m/s). A further increase in the injection speed leads to an increase in the wave velocity towards the flow of the freshly injected mixture. Note that the combustion of the propane-air mixture under the conditions under consideration is accompanied by a lower equilibrium temperature, compared to hydrogen-air and methane-air mixtures, and in almost the entire region ϕ subadiabatic temperatures are realized (Fig. 3b). Superadiabatic temperatures are possible only when the mixture composition is sufficiently saturated with fuel (the extreme point ϕ on the right (Fig. 3a))

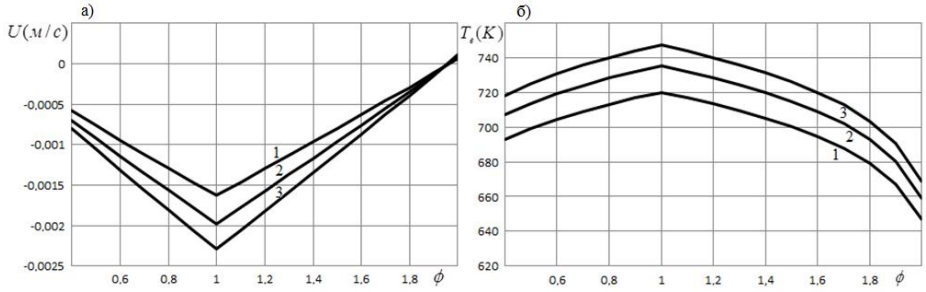

Figure 3.Curves of the dependence of the wave velocity (a) and the equilibrium temperature (b) of the propane-air mixture on the excess fuel coefficient with varying mixture injection speed: 1 — 0.52, 2 — 0.66, 3 — 0.79 m/s.

Calculations have shown that superadiabatic equilibrium temperatures during the combustion of a hydrogen-air mixture can be achieved by increasing the injection rate or significantly saturating the mixture with fuel. However, if the injection rate is increased sufficiently, superadiabatic equilibrium temperatures can be achieved even with fairly fuel-lean hydrogen-air mixture compositions. During methane combustion, superadiabatic equilibrium temperatures can be achieved both at low and relatively high injection rates, and at less saturated mixture compositions. The stationary wave of filtration combustion of a propane-air mixture has a counter-propagating motion for almost all the mixture compositions considered, and, as a result, is accompanied by subadiabatic equilibrium temperatures. According to the calculations, the co-propagating motion of the stationary wave is possible only for one propane-air mixture composition, corresponding to $\phi = 2$. Increasing the injection rate does not result in positive wave velocity values in other propane-air mixture compositions other than $\phi = 2$.

4. Conclusions

The calculations carried out using relations (4) and (6) lead to the following conclusions:

- the velocity of a stationary wave of a hydrogen-air mixture at low injection rates (from 0.1 to 0.5 m/s) has only negative values (of the order of 10^{-5} to 10^{-4} m/s), which corresponds to the counter-movement of the wave relative to the freshly injected mixture, and as a consequence, is accompanied by subadiabatic temperatures; an increase in the injection rate from 0.5 to 6 m/s increases the speed of the counter-movement of the wave to the order of 10^{-3} m/s, and contributes to the emergence of regions ϕ, where co-current wave motions are possible, which leads to the realization of superadiabatic equilibrium temperatures; positive values of the hydrogen-air mixture wave velocity, and as a consequence, superadiabatic equilibrium temperatures occur only at sufficiently saturated or too lean fuel mixtures;
- during combustion of a methane-air mixture, both co-propagation and counter-propagation of the combustion wave occur within the range of variation of the fuel excess ratio. Co-propagation (positive values) of the methane-air mixture wave velocity are realized in the fuel-lean region at relatively high injection velocities (starting from 0.6 m/s). In the fuel-rich region, the superadiabatic equilibrium temperature is realized at all injection velocities considered; the equilibrium temperature of the methane-air mixture is higher than for hydrogen-air and propane-air mixtures, and the superadiabatic temperature is realized in the fuel-rich region, at less saturated mixture compositions;
- for all considered propane-air mixture compositions and injection rates, the wave velocity values have negative values, except for one composition ($\phi = 2$), in which the velocity is positive at all injection rates considered. At this

composition, a superadiabatic equilibrium temperature is achieved, which is lower than the superadiabatic equilibrium combustion temperatures of hydrogen-air and methane-air mixtures.

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