Journal of Zhejiang University-SCIENCE A (Applied Physics & Engineering) 2022 23(10):838-844
www.jzus.zju.edu.cn; www.springer.com/journal/11582
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https://doi.org/10.1631/jzus.A2200217

Regimes of near-stoichiometric hydrogen/air combustion under reciprocating engine conditions

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1 Introduction

Hydrogen/air combustion is a problem both in respect of its fundamental science and in the use of hydrogen as a possible substitute for traditional hydrocarbon fuels. There is now a generally agreed approach to the use of hydrogen as an addition to traditional fuels (He et al., 2017) but the use of hydrogen as a main fuel has been studied much less because of the substantially unresolved problems for effective hydrogen production (Liu et al., 2020). It is worth noting that the use of hydrogen as a main fuel may be primarily applied not only for internal combustion engines needed for transport (Balat, 2008), but also for those serving as drives for electrogenerators within stationary power stations (Balat, 2008; Ivanov et al., 2018).

When studying hydrogen combustion under engine-like conditions the areas of knock and detonation occurrence are of primary interest (Zhao et al., 2019) since they represent undesirable processes for optimal engine operation. Such issues emerge when the ratio between hydrogen and oxidizer is close to stoichiometry but, at the same time, combustion proceeds more efficiently when the ratio between fuel and oxidizer is stoichiometric. It should be noted that we are not here considering detonation engines, where a hydrogen/air stoichiometric mixture is used and where detonation is the necessary means for engine operation (Lei et al., 2020). In a number of studies knock and super-knock are observed in hydrogen-fueled spark-ignition (Szwaja et al., 2007; Qi et al., 2015) and homogeneous charge compression ignition (HCCI) engines (Szwaja and Grab-Rogalinski, 2009; Pan et al., 2018). Some authors distinguish types of combustion regimes in engines as well as in constant volume chambers: "light" and "heavy" knock (Szwaja and Naber, 2013); normal and oscillating combustion, and end-gas autoignition (Wei et al., 2017); normal combustion without autoignition, autoignition without detonation, and detonation (Yu and Chen, 2015).

Despite some research interest on their problems, the combustion processes of near-stoichiometric hydrogen/air mixtures in internal combustion engines have not been investigated enough. There is no systematic understanding of the conditions for the onset of different combustion regimes and there is almost no information on the particular mechanisms responsible for knock in the hydrogen/air mixture under spark-ignition engine conditions. Also, it should be noted that experimental analysis as a rule does not provide enough information for detailed analysis of the particular physical mechanisms responsible for establishment of one or another mode of combustion. Therefore, mathematical modeling is the route to improved understanding of the processes developed inside the combustor under the conditions of interest.

In the present work, we study numerically the combustion of near-stoichiometric hydrogen/air mixtures inside a cylindrical chamber under a moving piston with the initial conditions and parameters relevant to a reciprocating engine with spark ignition. The initial cylinder chamber of 1.86 L undergoes a compression ratio of 11.4 under the moving planar piston. The spark is modeled as an additional energy input of 17 mJ in a small region on the top of cylinder. A detailed description of the problem setup is presented in the electronic

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Received Apr. 19, 2022; Revision accepted May 23, 2022; Crosschecked Aug. 31, 2022

supplementary materials. The main attention is paid to a detailed analysis of flame front dynamics which enables a deeper insight into combustion development and the associated pressure oscillations and so gives a true understanding of the regime that occurs in the engine and whether it differs from knock in its origin.

2 Results and discussion

2.1 Results of numerical simulations

We consider combustion regimes with hydrogen/air mixtures of stoichiometric (29.5% of hydrogen by volume) and sub-stoichiometric (less than 29.5%) compositions in the combustion chamber with parameters presented in the electronic supplementary materials. Pressure histories obtained numerically for combustion regimes of hydrogen/air mixtures of different compositions (29.5%, 26.0%, 24.0%, 22.0%, 20.0%, and 18.0%) are presented in Fig. 1a. Analysis of the data enables three characteristic combustion regimes to be distinguished: (1) detonation, observed for the stoichiometric mixture and originating spontaneously as a result of ignition of the compressed mixture, (2) a fast combustion regime, distinctively observed in the 26.0% (as well as in the 24.0% and 22.0%) mixture where the pressure history is characterized by pressure oscillations of relatively high amplitude and frequency, and (3) a slow combustion regime, realized for 18.0% hydrogen content in the mixture, where the pressure history is characterized by pressure oscillations of relatively low amplitude.

Histories of heat release rates corresponding to combustion regimes in mixtures with different hydrogen contents are shown in Fig. 1b. For the detonation regime, this curve degenerates into a single spike indicating the fast burning of the whole mixture inside the combustion chamber in a supersonic detonation wave.

Figs. 2 and 3 depict characteristic flow fields corresponding to all the selected combustion regimes. A clear distinction of different regimes can be observed not only from the indicator diagrams but also from the analysis of flow pattern evolution (Figs. 2 and 3). The fast combustion regime is characterized by a fast-propagating and highly distorted flame front, while the slow combustion regime is characterized by a smoother pattern of flame development.

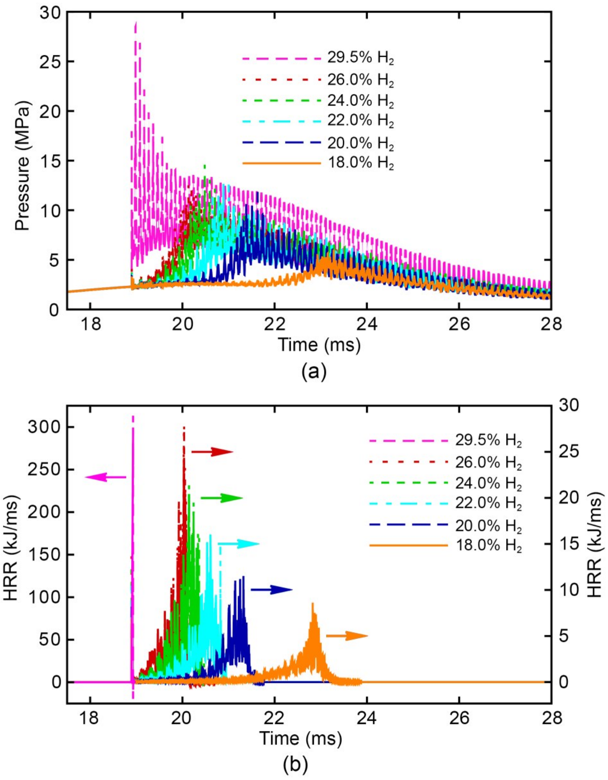

Fig. 1 Pressure (a) and heat release rate (HRR) (b) histories for different initial hydrogen contents in its mixture with air

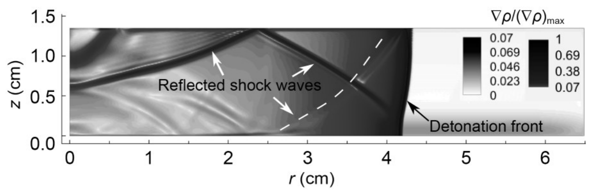

Fig. 2 Normalized density gradient (∇*ρ*) field for detonation burning of 29.5% (in volume) H_2 in air at the time instant of 18.92 ms from the start of a compression stroke (through 29 μs after the start of spark ignition). Bottom boundary: piston; upper and right boundaries: cylinder walls; left boundary: symmetry axis. *r* and *z* are cylindrical coordinates (radius and height, respectively)

In these conditions, the adiabatic compression (11.4 times) of a combustible hydrogen/air mixture (adiabatic index γ=1.4) under the piston corresponds to the rise of pressure and temperature of the mixture up to 2.3 MPa and 686 K, respectively, at the time instant when the ignition is initiated (18.89 ms). The ignition of the stoichiometric mixture under these conditions from the energy source of 17 mJ leads to the formation of a detonation wave (in Fig. 2 it propagates from left to right at 1821 m/s). This regime is of interest due to the fact that the knock regime in

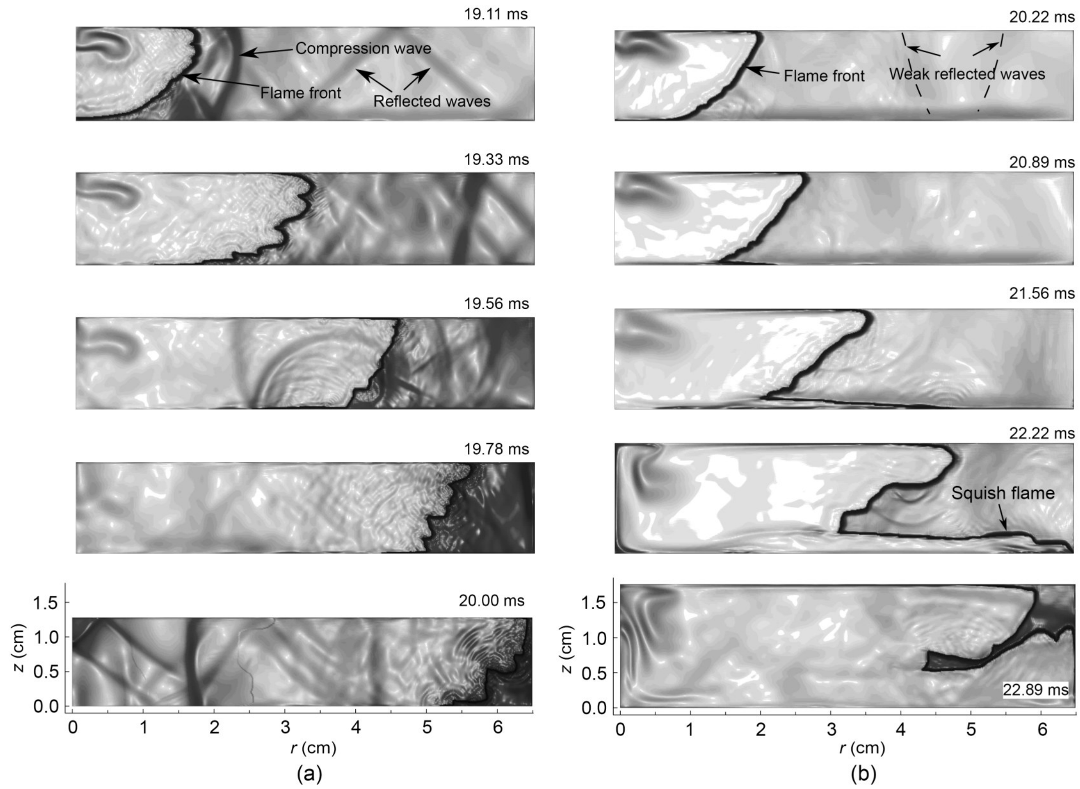

Fig. 3 Normalized density gradient fields during combustion of 26.0% (in volume) H_2 (a) and 18.0% H_2 (b) in air. Bottom boundary: piston; upper and right boundaries: cylinder walls; left boundary: symmetry axis. The 20.00 ms corresponds to the end of compression. The time intervals between plots are 0.22 ms (a) and 0.67 ms (b)

engines is associated, as a rule, specifically with detonation wave formation after its initiation from the hot spot formed in the end-gas region ahead of the main flame front (Qi et al., 2015; Wang et al., 2017; Filimonova et al., 2020). After the whole fuel-air mixture in the combustion chamber is burned, the detonation wave degenerates into a shock wave propagating through the combustion products.

In Fig. 3, density gradient fields are presented for the fast and slow combustion regimes formed in 26.0% and 18.0% of H_2/air mixtures, respectively. It should be noted that the color map, i.e. the correspondence of color tones to certain values of density gradient, is the same for Figs. 2 and 3; that is necessary for visual comparison of flow patterns in these cases. The more intensive combustion of the 26.0% mixture and, therefore, the faster flame propagation from the ignition source result in the generation of compression waves reflecting from the chamber walls and affecting the flame front. At the early stages of combustion, the reflections of compression waves from the chamber walls are represented on the pressure history as relatively low-pressure oscillations at the background of a monotonic pressure rise resulted from the burning mixture. The interaction of the compression waves with the flame front promotes the enhancement of its gas-dynamic instability. Thus, the comparison of flame surfaces for two regimes (Figs. 3a and 3b) indicates that in the case of the 26.0% mixture, the front surface turns out to be significantly more wrinkled. Here, it is worth noting that the gas-dynamic instability of the flame front itself in the more intensively reacting mixture develops faster (an increment of instability rise at the linear stage is $\alpha \sim u_f/\lambda$, where u_f is the normal burning rate, and λ is the perturbation wavelength (Lifshitz and Landau, 1987)). Impact of compression waves on the perturbed flame front promotes a change in the velocities of certain front regions and additional flame stretching that represents a complementary factor of amplification of instability development. Another important factor of the interaction of the compression wave with the developed flame front surface is its amplification by the following mechanism: when the compression wave passes the zone of energy release (the flame front), it is intensified naturally (Yang et al., 2013; Kiverin and Yakovenko, 2021). This factor can be explicitly observed when analyzing the pressure history, where a rise of pressure oscillation amplitudes against a monotonic rise of pressure is observed (Figs. 1 and 5). Herewith, one can clearly see that both pressure and heat release fluctuations are in phase; that illustrates the above formulated mechanism and corresponds to the conventional definition of thermoacoustic instability. Upon the realization of a slow combustion regime in a lean mixture (18.0%), this rise of pressure oscillation amplitude is less expressed. When the front of the fast flame (Fig. 3a) approaches the cylinder side-wall, the flame front locally takes the shape of sharp peaks that facilitate an additional focusing of the compression waves and enhance their impact on the chamber walls and piston surface. Note that, in the case of the slow combustion regime, complete combustion is achieved during the expansion stage.

Fig. 4 shows the temperature field in the end-gas region at time instants directly before the combustion termination. These patterns show clearly that the temperature in the end-gas region is not higher than 690 K for the detonation regime (a), 900 K for the fast combustion regime (b), and 800 K for the slow combustion regime (c). This demonstrates that hydrogen autoignition in the end-gas region is not possible for each of the variants (a)–(c) since the ignition delay at the observed temperatures is much longer than the time of the flame approaching the wall. We also have performed simulations analogous to those presented above, but with higher compression ratios, 14.0 and 20.0 for 29.5% and 22.0% hydrogen contents, respectively. In those cases there is also no autoignition of the end-gas observed, as the temperature of the end-gas is not sufficient.

Now we analyze pressure oscillations developing in the process of combustion and after its termination, for three combustion regimes. Fig. 5a presents histories of pressure amplitudes obtained in the following way. First, we take the average approximation for the pressure histories and then we subtract these mean curves from the initial ones. The comparison of detailed elements of the indicator diagrams at the expansion stage, after combustion completion (Fig. 5b), shows that the characters of oscillations for different regimes are distinct. With the decrease in combustion intensity, from detonation to a slow combustion regime, the amplitude and frequency of the oscillations

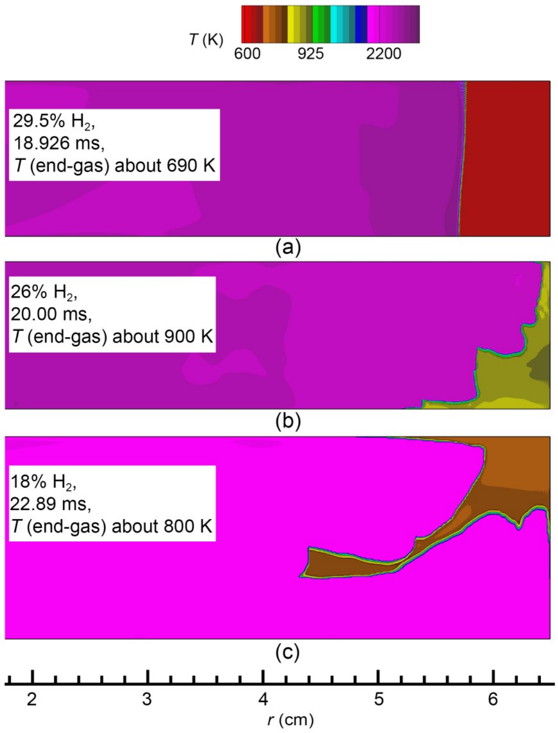

Fig. 4 Temperature fields at time instants prior to the combustion termination for the detonation regime (a), fast combustion regime (b), and slow combustion regime (c). Bottom boundary: piston; upper and right boundaries: cylinder walls

decrease. In Fig. 5c, results of fast Fourier transform are presented, while the obtained functions of frequency are not normalized. The data presented here demonstrate that the frequencies of corresponding peaks for the three regimes shift to higher values from the slow combustion regime to detonation. This is explained by the nature of the pressure oscillations, as shown in Fig. 5b.

Furthermore, their frequency can be estimated by the characteristic speed of the arising compression waves divided by the characteristic size of the combustion chamber (its diameter). As the latter is considered equal for each combustion regime, the frequency will depend mainly on the speed of the arising compression wave, which in turn is defined by the intensity of the combustion regime. Therefore, for the more intense combustion regime, the frequency is higher than for the less intense one.

We now consider the nature of pressure oscillations for each combustion regime. In the case of detonation, pressure oscillations relate to the development of a strong shock wave in the chamber volume as a

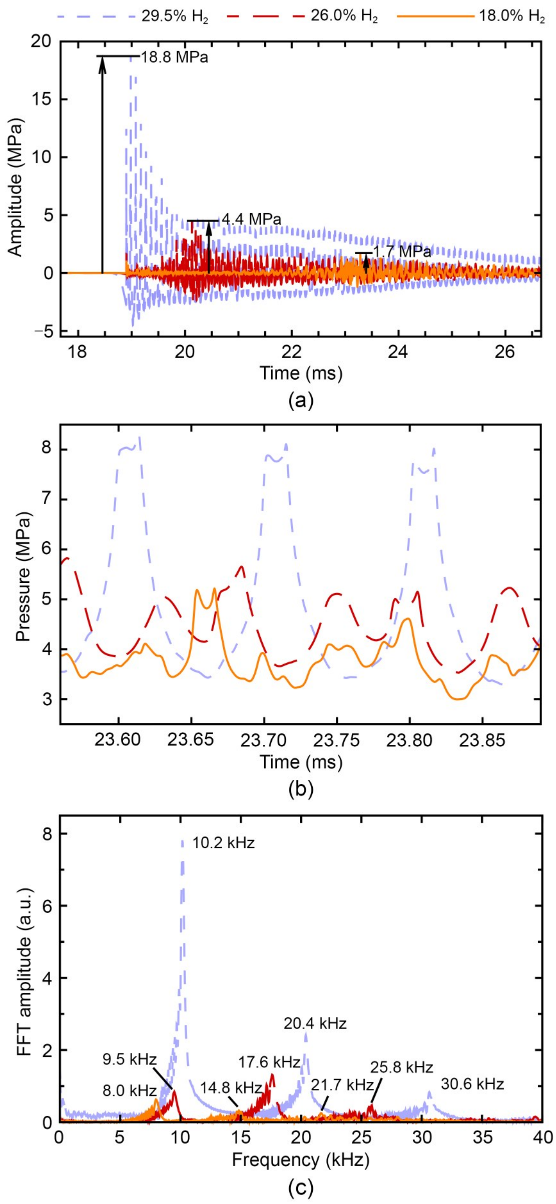

Fig. 5 (a) Pressure amplitudes for three different combustion regimes; (b) magnified fragments of pressure histories from Fig. 1a; (c) results of fast Fourier transform (FFT) of dependencies (a)

result of detonation degeneration after the burning of the whole mixture. In the case of fast combustion, the pressure oscillations are associated with the generation of relatively strong compression waves amplified at the stage of combustion development by the mechanism of thermoacoustic instability. In the case of slow combustion, the amplitude of the compression waves is low, and pressure oscillations are mostly expressed by pressure oscillations of burned gas inside the chamber caused by the non-uniform character of mixture burning and the generation of a corresponding flow field.

2.2 Comparison of the fast combustion regime with knock regimes in spark-ignition engines

We have observed that the pressure histories and pressure oscillation spectra for the fast combustion regime are similar to those where the knock event is observed (Szwaja et al., 2007; Qi et al., 2015; Pan et al., 2018). However, knock in spark-ignition engines is usually associated with the autoignition of unburned mixture in the end-gas region ahead of the propagating flame front and a subsequent detonation wave formation (Heywood, 1988; Wang et al., 2017). The main causes of knock in spark-ignition engines are (Wang et al., 2017): surface ignition due to the heated chamber elements, ignition by hot spots which could be oil particles or carbon particles, heating by the pressure and shock waves generated by an intensively propagating flame front and reflected from the chamber walls, and the effect of the low temperature combustion of some fuels expressed by the existence of a temperature range where the induction time decreases with the temperature decrease (negative temperature coefficient, NTC).

The kinetics of hydrogen combustion does not have such features as NTC unlike many hydrocarbon fuels, and thus that cause of knock is not present in the case of hydrogen. Causes associated with the surface ignition and ignition by hot spots are external relative to the reacting mixture. Therefore, the only possible cause of knock determined by the dynamics and properties of the hydrogen/air mixture is the influence of pressure waves generated by the flame front propagation within the enclosed volume.

The present investigation shows that even under highly intensive combustion development and in the presence of pressure waves of significant amplitude (detonation and fast combustion regimes), the autoignition of hydrogen ahead of the flame front does not occur. As Fig. 4 demonstrates, the temperature of 900 K (and pressure of 7.46 MPa) for the fast combustion regime in the end-gas region corresponds to an induction time of 24.6 ms. That time is more than two orders of magnitude higher than the characteristic time of mixture burning in the end-gas region due to flame propagation. According to the performed simulations (Fig. 3a), combustion of the mixture in the end-gas region at the final stage of the process proceeds for 0.1 ms.

3 Conclusions

In the present study, 2D numerical simulations of combustion gas dynamics in near-stoichiometric hydrogen/air mixtures filling the chamber under compression by a piston were performed. With the decrease in initial hydrogen content in its mixture with air (air-to-fuel equivalence ratio of 1.0–1.9), three combustion regimes are obtained: detonation, a fast combustion regime, and a slow combustion regime. Detailed insight into the flame front shape during hydrogen combustion under reciprocating engine conditions at different initial hydrogen contents is obtained. The regimes of detonation and fast combustion can lead to high dynamic loads as well as heating of the chamber and piston elements. The regime of fast combustion differs from the regime of slow combustion by a more intensive development of gas-dynamic instability of the flame front under the interaction of the flame with compression waves inside the enclosed combustion chamber. The regime of fast combustion is similar to knock according to its output parameters. However, this regime is not knock in the traditional understanding of this term since, despite the high intensity of pressure waves generated by the flame and amplified by the mechanism of thermoacoustic instability, autoignition of the mixture ahead of the flame front does not occur.

Acknowledgments

This work is supported by the Ministry of Science and Higher Education of the Russian Federation (No. 075-15-2020-806).

Author contributions

Alexey D. KIVERIN designed the research. Anna E. SMYGALINA processed the corresponding data. Anna E. SMYGALINA wrote the first draft of the manuscript. Alexey D. KIVERIN revised and edited the final version.

Conflict of interest

Anna E. SMYGALINA and Alexey D. KIVERIN declare that they have no conflict of interest.

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Electronic supplementary materials

Section S1