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

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Key words: hydrogen, combustion, detonation, pressure oscillations, stoichiometry, numerical modeling

Aims of this study

Combustion processes of near-stoichiometric hydrogen/air mixtures in internal combustion engines have been investigated rather **insufficiently** and there is **no systematic understanding of the conditions for different combustion regimes onset** as well as there is almost no information on the particular **mechanisms responsible for knock** in hydrogen/air under spark ignition engine conditions.

In the present work:

- We study numerically combustion of near-stoichiometric hydrogen/air mixtures inside the cylindrical chamber under the moving piston with the initial conditions and parameters relevant to reciprocating engine with spark ignition.
- The main attention is paid to the **detail analysis of flame front dynamics** that enables to give deeper insight into combustion development and associated pressure oscillations and to understand truly what kind of regime occurs in engine and whether it differs from knock in its origin.

Mathematical model and numerical algorithm

• Mathematical model: **Navier – Stokes** gas-dynamic system of equations with account of viscosity, multicomponent diffusion, thermal conductivity and heat release due to chemical reactions.

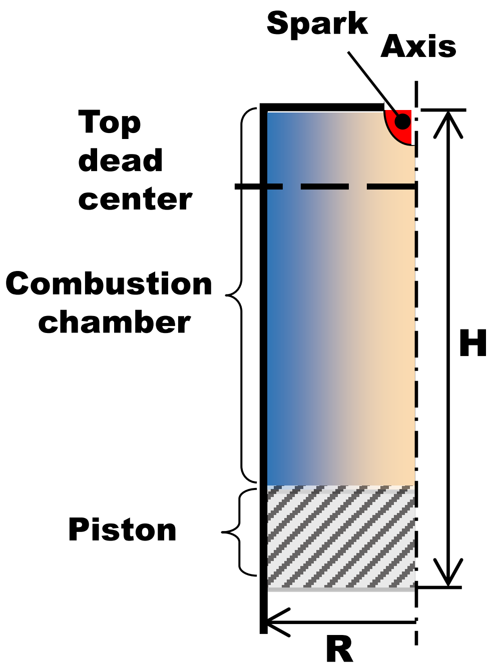
• In order to resolve the gas-dynamic system of equations numerically the Euler – Lagrangian method (**method of “coarse particles”**) was used. This method has 1^{st} order of accuracy in time and 2^{nd} one in space.

• The resolution is carried out in **2D setup in cylindrical coordinates** with account of axial symmetry.

• The modelling of chemical transformation is realized using the **detail mechanism of chemical kinetics** [*O Conaire et. al. Int. J. Chem. Kinet. 2004. Vol. 36 (11). P. 603-622*], consisting of 21 reversible reactions between 8 components (N_2 was regarded as neutral component).

• The mathematical model used enables to obtain qualitatively as well as quantitatively **accurate results** (while comparing with experimental data) for different combustion regimes: **deflagration, detonation and ignition processes** (*Ivanov et al. Int. J. Hydrogen Energy 2013. Vol. 38. P. 16427-40, Ivanov et al. Int. J. Hydrogen Energy 2017. Vol. 42. P. 11902-10*)

Problem setup

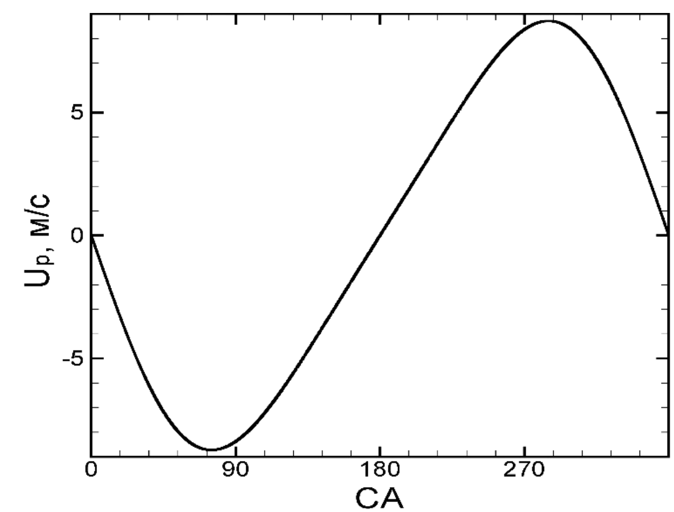


Cylinder height (H)	14 cm
Cylinder radius (R)	6,5 cm
Compression ratio	11,4
Crankshaft rotational speed (ν)	1500 rpm
Spark timing	18,89 ms (10 CAD bTDC)
Spark energy	17 mJ
Spark duration	12 μs

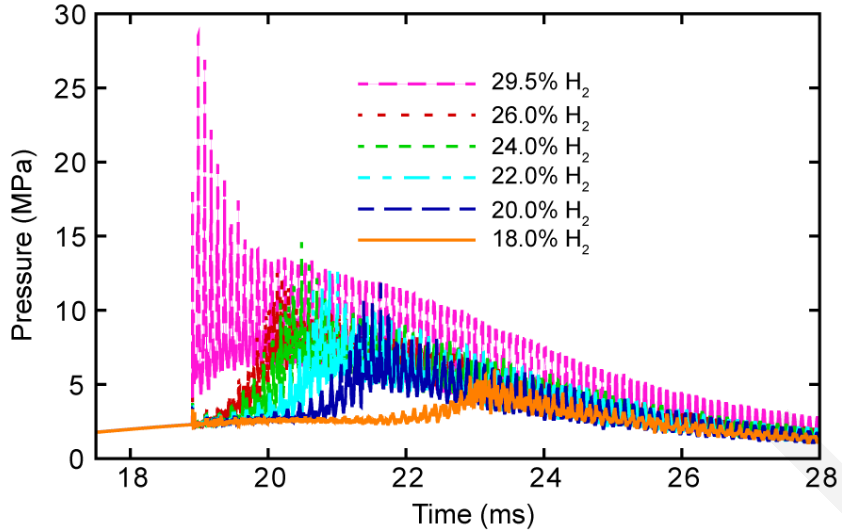
- Chamber and piston walls were regarded **adiabatically isolated**.
- Spark ignition was modelled as an **additional energy input**.

Piston moves in the cylindrical chamber, filled with combustible mixture, at speed determined by kinematic relation

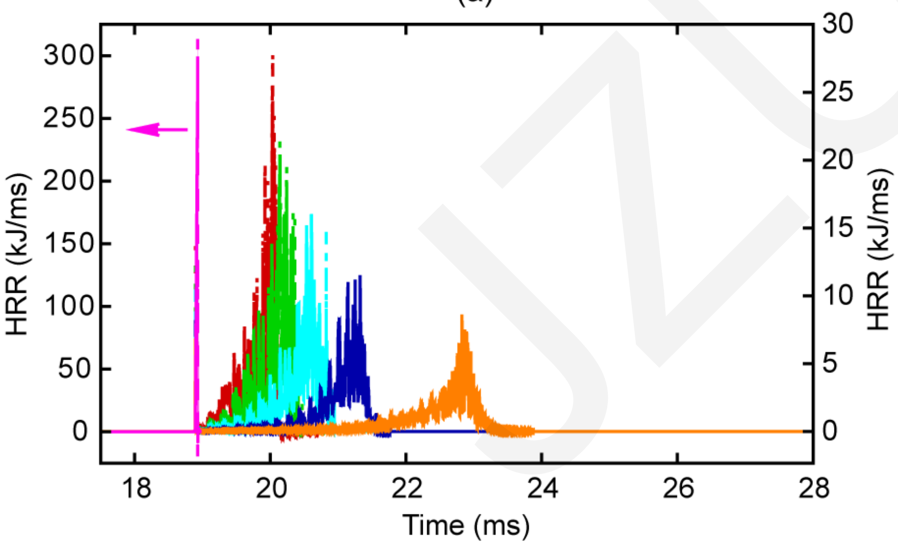
$$U_p = U_0 \frac{\pi}{2} sin(2\pi\nu t)\left(1 + \frac{cos(2\pi\nu t)}{\sqrt{16 - sin^2(2\pi\nu t)}}\right)$$



Indicator diagrams



(a)



(b)

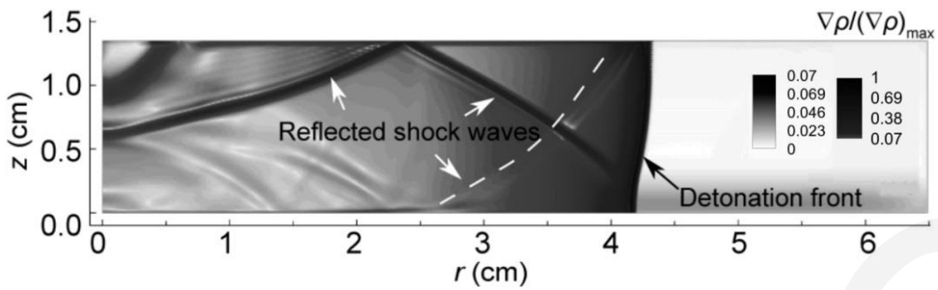
Analysis of indicator diagrams enables to distinguish three characteristic combustion regimes:

1)detonation, observed for stoichiometric mixture and originating spontaneously as a result of ignition of compressed mixture,

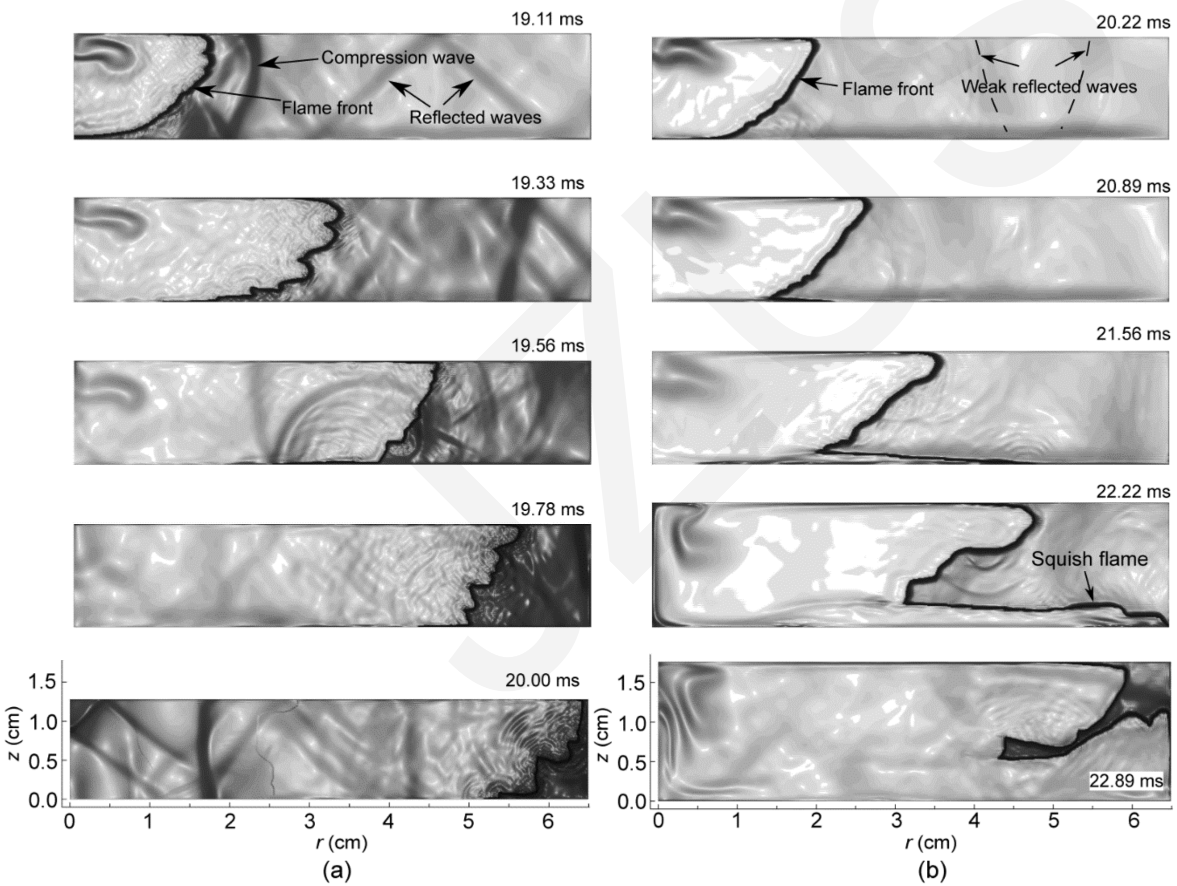
2)fast combustion regime, distinctively observed in the 26.0% (or 24.0%, or 22.0%) mixture: here the indicator diagram is characterized by pressure oscillations of relatively high amplitude and frequency, and

3)slow combustion regime, realized for 18.0% hydrogen content in the mixture: indicator diagram is characterized by pressure oscillations of relatively low amplitude.

Combustion regimes: detonation, fast and slow combustion

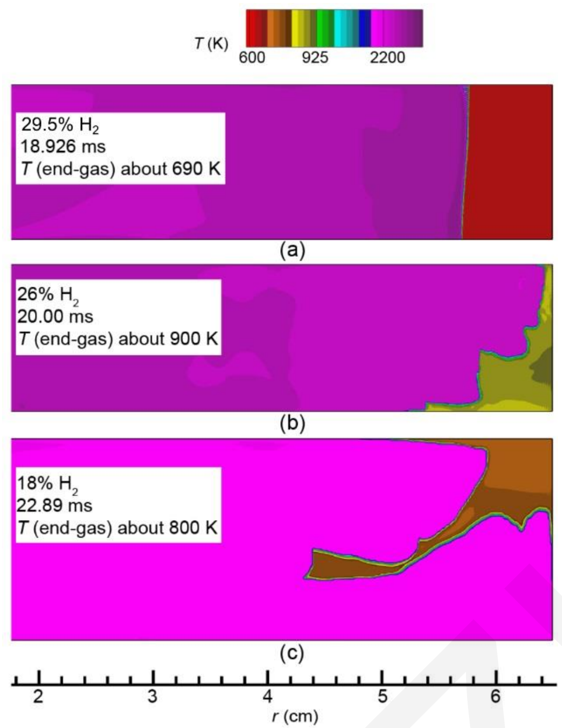


- **Density gradient field for the detonation regime, occurred for stoichiometric H_2/air mixture**



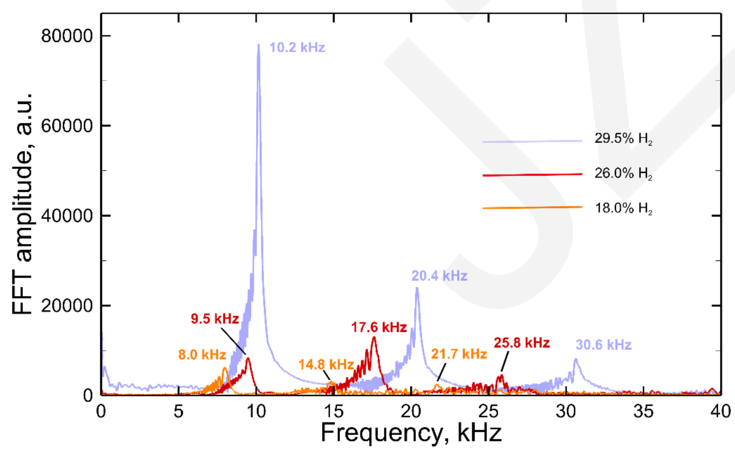
- **Density gradient fields for the fast (a) and slow (b) combustion regimes, occurred for 26.0% (vol.) H_2/air mixture and 18.0% (vol.) H_2/air mixture, correspondingly.**

Analysis: causes of knock in hydrogen engine



Temperature fields for the moments, when combustion terminates (Bottom boundary – piston, upper and right boundary – cylinder walls).

Figure shows that the temperature of the end-gas for the moments when combustion terminates is not higher than 690 K for detonation regime (a), 900 K for fast combustion regime (b), and 800 K for slow combustion regime (c). For the moments less than considered ones the temperature is even less than the values presented. This demonstrates that the auto-ignition of the end-gas is not possible for each of the variants (a)-(c).



Results of fast Fourier transform (FFT) of pressure amplitude histories.

The fast combustion regimes of hydrogen in the chamber under the moving piston in SI engine are **similar to knock regimes** observed in the process of combustion of different fuels, including hydrogen.

The term knock in SI engine is usually associated with the **auto-ignition of end-gas**.

In the present investigation it is shown that even under highly intensive combustion development and the presence of pressure waves of significant amplitude (detonation and fast combustion regimes), the auto-ignition of hydrogen ahead of the flame front does not occur.

Conclusion

1. With the decrease of initial hydrogen content in its mixture with air (λ = 1.0 – 1.9) three combustion regimes are obtained: **detonation, fast combustion regime and slow combustion regime**.

2. The regime of fast combustion differs from the regime of slow combustion by more intensive development of **gasdynamic instability** of the flame front under the interaction of flame with compression waves inside the enclosed combustion chamber volume.

3. The regime of **fast combustion is similar to knock** according to its output parameters, however, this regime is not knock in traditional understanding of this term since **the auto-ignition of mixture ahead of the flame front does not occur**.