

Electronic Supplementary Materials

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

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S1 Problem setup

To analyze the features of hydrogen combustion under the reciprocating engine conditions the following problem setup is considered (fig. 1). The cylinder chamber of 1.86 liter volume is filled with hydrogen/air mixture. The bottom wall of the chamber represents a moving piston which starts its motion at initial time instant and causes mixture compression by 11.4 times. The compression is assumed to be adiabatic that causes corresponding rise in temperature and pressure of the mixture. The law of piston motion is taken from [Heywood, 1988] and is written in the following form

$$S_p = S_0 \frac{\pi}{2} \sin(2\pi\nu t) \left(1 + \frac{\cos(2\pi\nu t)}{\sqrt{A^2 - \sin^2(2\pi\nu t)}} \right),$$

where S_0 – mean piston velocity determined by the piston stroke and the rotational speed of the crankshaft, - 6.34 m/s; ν – rotational speed, 1500 rpm; A – ratio of connecting rod length to crank radius, 4.0. The compression stroke takes 20 ms. The start of compression corresponds to 0 ms, the end of compression – to 20 ms.

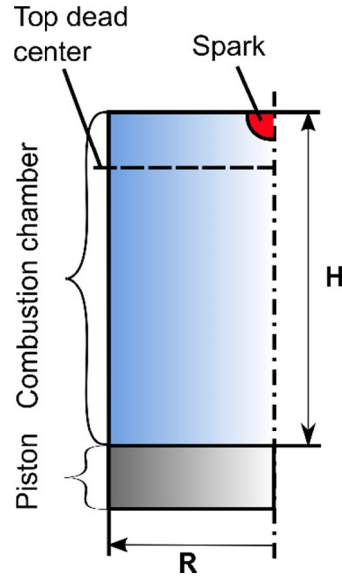


Fig. S1 Problem setup.

The mixture is ignited with an energy source located in the central part of the top wall of the chamber at 10 crankshaft angle degrees before the top dead center (at time instant 18.89 ms from the compression start). Further the combustion wave is formed and propagates inside the chamber at the background of piston motion. To observe different regimes of combustion development the initial mixture composition is varied from stoichiometric down to lean composition. Simulations of dynamics and combustion of a hydrogen/air gaseous mixture under compression and expansion inside the combustor are conducted in 2D axisymmetric setup in cylindrical coordinates (r, z) . The employed mathematical model represents a compressible Navier – Stokes system of equations with account of viscosity, thermal conductivity, multicomponent diffusion and chemical conversion processes. The system of equations in axisymmetric form is written as follows:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial(\rho r u_r)}{\partial r} + \frac{\partial(\rho u_z)}{\partial z} &= 0, \\
\rho \left(\frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + u_z \frac{\partial u_r}{\partial z} \right) &= -\frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial(r \sigma_{rr})}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z}, \\
\rho \left(\frac{\partial u_z}{\partial t} + u_r \frac{\partial u_z}{\partial r} + u_z \frac{\partial u_z}{\partial z} \right) &= -\frac{\partial p}{\partial z} + \frac{1}{r} \frac{\partial(r \sigma_{zr})}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z}, \\
\rho \left(\frac{\partial w_s}{\partial t} + u_r \frac{\partial w_s}{\partial r} + u_z \frac{\partial w_s}{\partial z} \right) &= \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho D_s \frac{\partial w_s}{\partial r} \right) + \frac{\partial}{\partial z} \left(\rho D_s \frac{\partial w_s}{\partial z} \right) + M_s r_s, \\
\rho \left(\frac{\partial E}{\partial t} + u_r \frac{\partial E}{\partial r} + u_z \frac{\partial E}{\partial z} \right) &= -\frac{1}{r} \frac{\partial(r p u_r)}{\partial r} - \frac{\partial(p u_z)}{\partial z} + \frac{1}{r} \frac{\partial(r \sigma_{rr} u_r + r \sigma_{rz} u_z)}{\partial r} + \\
&\quad + \frac{\partial(\sigma_{zr} u_r + \sigma_{zz} u_z)}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \kappa \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(\kappa \frac{\partial T}{\partial z} \right) + \\
&\quad + \sum_{k=1}^N h_k \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \rho D_k \frac{\partial w_k}{\partial r} \right) + \frac{\partial}{\partial z} \left(\rho D_k \frac{\partial w_k}{\partial z} \right) \right) - \sum_{k=1}^N h_k r_k,
\end{aligned}$$

where u_r, u_z – velocity projections on r, z reference axes; w_s – mass fraction of species s ; E – total energy of the unit of mass fraction of gas; p, ρ, T – pressure, density and temperature, correspondingly; σ – viscosity tensor; D_s – diffusion coefficient; κ – thermal conductivity coefficient; r_s – velocity conversion of molar fraction of

species s in the process of chemical transformation; M_s – molar mass of species s ; h_k – molar enthalpy of species k ; N – number of species.

The gas-dynamic system of equations is solved numerically using modified Eulerian – Lagrangian method [Lieberman *et al.*, 2004; Lieberman *et al.*, 2006], having 2nd order of accuracy in space and 1st one in time. Coefficients of molecular transport processes are calculated according to relations presented in [Warnatz *et al.*, 2001]. Hydrogen oxidation is modeled using the detailed mechanism of chemical kinetics [O Conaire *et al.*, 2004], containing 21 reversible reactions between 8 species. N₂ molecule is involved in chemical conversion only as a third body; the process of nitrogen oxidation in this study is not taken into account.

The numerical algorithm presented enables to obtain qualitatively as well as quantitatively reliable results for different combustion regimes. This algorithm was repeatedly applied for modelling of combustion in spark-ignition engines [Ivanov *et al.*, 2018; Lieberman *et al.*, 2004; Lieberman *et al.*, 2006; Zaichenko *et al.*, 2018]. Furthermore, in [Lieberman *et al.*, 2004; Lieberman *et al.*, 2006; Zaichenko *et al.*, 2018] a favourable agreement with experimental results was obtained that serves for a validation of the algorithm in solving such a class of problems. Thus, for example in [Zaichenko *et al.*, 2018], when modeling combustion of hydrogen/air mixture with air-to-fuel equivalence ratio of 1.5 the error in numerical determination of the full duration of combustion compared with the experimental data was obtained to be less than 1% (numerical and experimental values were ~1.49 ms). In case of air-to-fuel equivalence ratio of 2.0 the error was 19% (1.67 ms numerical, 1.99 ms experimental).

At the initial time instant the chamber is filled with hydrogen uniformly premixed with air. The hydrogen content is varied in the range from 29.5% (by volume; throughout the paper % designates % vol.) down to 18.0% for a certain simulation and corresponds to air-to-fuel equivalence ratio λ varied from 1.0 up to 1.9. The initial velocity of mixture in the whole volume of the combustion chamber is set equal to zero. The initial temperature and pressure are 300 K and 0.1 MPa, respectively. The domain of combustion chamber is assumed adiabatically isolated, and the non-slip condition is set at its inner boundaries.

The spark ignition is modelled as an additional energy input during 12 μ s into the region of 0.4 mm radius located at the center of the chamber on its top end wall. The sum spark energy is equal to nearly 17 mJ and the start of ignition is set at the time instant corresponding to 18.89 ms for each simulation.

The initial height (H) and the radius (R) of the chamber are 0.14 m and 0.065 m, correspondingly (fig. 1). The space grid is uniform, the cell size is chosen equal to 100 μ m that is sufficient for conducting the analysis of flame dynamics and front shape. Convergence test is carried out in the range of cell sizes from 400 μ m down to 50 μ m. The full duration of the burning process is used as a test parameter, and it is found that rate of convergence (calculated according to the Richardson' routine [Roache, 1994]) at 100 μ m equals to 1.89 that shows sufficient degree of convergence and possibility to use this resolution for accurate computations. The error relative the estimated exact solution at 100 μ m cell size is 18% while it goes down to 5% at 50 μ m cell size. Nevertheless, all the peculiarities of flame evolution and pressure oscillations are reproduced well enough at 100 μ m cell size and the following calculations are carried out using it.

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