3D simulation of hydrogen ignition in a rapid compression machine

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Low-temperature (at T < 900–950 K) ignition delays of hydrogen–air mixtures are mainly measured in rapid compression machines (RCM). This communication is aimed at numerical simulation of ignition delays of hydrogen–air mixtures in the RCM by means of a coupled three-dimensional (3D) Unsteady Reynolds-Averaged Navier–Stokes (URANS) — Particle Method (PM) simulation of RCM operation capable of catching turbulence–chemistry interaction. The study indicates that the time history of piston motion in an RCM affects the final state of a test mixture at the end of compression stroke and therefore influences the phenomena relevant to test mixture ignition. More specifically, the calculations show that different laws of piston motion at a fixed average piston velocity (i.e., fixed piston displacement and fixed compression time) and fixed compression ratio result in different evolution of mean pressure, temperature and velocity fields in the RCM test section leading to different ignition behavior. The reasons for the arising differences lie in the fact that the local instantaneous piston velocity determines the roll-up vortex structure, strength and turbulence dissipation in it, heat transfer in test-section walls, and mass leakage through piston rings.

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1. Introduction

In the industrial process safety there is growing understanding of the importance of spontaneous ignition phenomena in the course of accident evolution. Spontaneous ignition of a reactive medium can occur at uncontrolled mixing of fuel and oxidizer jets, at reflections of blast waves from confining walls or obstacles, behind a lead shock wave generated by a high-speed turbulent flame propagating in a long pipeline, and in many other situations. Of particular interest is the explosion accident scenario with generation of relatively low-intensity pressure waves that can nevertheless produce significant damage due to pressure buildup caused by spontaneous volumetric ignition after wave reflections. Such pressure waves can accompany transient combustion processes propagating with the visible flame velocities higher than several tens of meters per second.

Spontaneous ignition is characterized by the ignition delay, the time taken for reactive mixture to self-ignite after it is subjected to preset thermodynamic conditions. Ignition delays are usually measured in shock tubes and in rapid compression machines (RCM). Because of a limited maximum measurement time on the order of 1–2 ms, Gaydon and Hurle (1963), shock tubes are in general not applicable for studies of low-temperature self-ignition phenomena relevant to the aforementioned accidental explosion scenario with low-intensity pressure waves. As for RCM, this device is intensely used to measure ignition delays of various gaseous explosive mixtures in the entire millisecond range, i.e., at relatively low reference temperatures (Affleck & Thomas, 1968; Beeley, Griffiths, & Gray, 1980; Donovan et al., 2005; Cersen, Anikin, Mokhov, & Levinsky, 2008; Griffiths et al., 1993; Lee & Hochgreb, 1998; Leshevich & Penyazkov, 2011; Minetti, Ribaucour, Carlier, Therssen, & Sochet, 1995; Mittal, Sung, & Yetter, 2006; Park & Keck, 1990). In view of it, better understanding of the specific features of RCM operation and their effect on the measured ignition delays is important.

Fig. 1 shows the schematic of the flat-piston head RCM with the piston assembly. The RCM is composed of the test, driver, and buffer sections with the corresponding parameters denoted by indices 1, 2, and 3. The test section is initially filled with the ignitable test gas at initial pressure and temperature $p_0$ and $T_0$ whereas the driver section is filled with a driver gas at elevated initial pressure. The test and driver gases are separated with the piston assembly of total mass $m$. After activating a special trigger at time $t = 0$, the piston assembly gets in motion with time-variable velocity $v_p(t)$ and the...
test gas undergoes compression accompanied with pressure, temperature and density increase. After a preset displacement $\Delta l$ (limited by a piston stopper), the piston stops. The time of piston motion (compression time) is further denoted as $t_c$. The buffer section is needed to control piston motion and to avoid piston oscillations upon stopping. At certain conditions, the compressed test gas can spontaneously ignite. The ignition time is further denoted as $t_{\text{ign}}$.

The ignition event in the test section is usually registered applying various optical and pressure-sensing techniques. To better identify the ignition conditions in terms of instantaneous pressure $p_1$ and temperature $T_1$, ignition in the standard procedure is required to occur after the piston stops. In view of it, the most important parameter of the RCM is the compression ratio $\beta = (l_1 + \Delta l)/l_1$, where $l_1$ is the length of the test section when the piston has reached its final position (see Fig. 1). The compression ratio is used to estimate $p_1$ and $T_1$ irrespective of the piston motion history determined by $v_p(t)$, $m$ and $t_c$, and the actual heat balance. The main measured parameter in the RCM is the ignition delay time $t_{\text{ign}} = t_{\text{ign}} - t_c$.

The survey of relevant literature indicates that the absolute values of ignition delays of hydrogen–air or hydrogen–oxygen–diluent mixtures measured using such a standard procedure can differ by up to one order of magnitude for seemingly very similar sets of thermochemical parameters $p_1$ and $T_1$ at $t = t_c$. As an example, Fig. 2 shows the measured ignition delays on temperature and pressure for hydrogen containing gaseous mixtures obtained in RCM by different authors. The observed discrepancies are often attributed to the RCM design and construction materials, as well as to different piston and test section geometries in the corresponding literature sources.

This paper is aimed at finding other possible reasons of observed discrepancies in measured ignition delays of hydrogen–air mixtures in the RCM. One of these reasons is the difference in the piston velocity history during experiments with apparently similar ignition conditions in terms of mixture pressure $p_1$ and temperature $T_1$ after compression. As follows from the above description, the standard procedure of measuring ignition delay $t_{\text{ign}}$ does not take into account the history of piston motion. However one can readily note a number of accompanying physical phenomena which potentially affect the value of $t_{\text{ign}}$.

First, note that piston motion induces a toroidal roll-up vortex in the ignitable gas (Fig. 3). This vortex was detected in experiments of Daneshyar, Fuller, and Deckker (1973) and in numerical simulations of Griffiths et al. (1993) and Wurmel and Simmie (2005). Vortex strength and turbulence dissipation in it are obviously dependent on $v_p(t)$.

Second, note that test gas compression by the moving piston is accompanied with a gradually growing difference between the ignitable gas temperature $T_1$ and the temperature of test-section wall $T_w$, leading to time-variable heat transfer to the RCM walls. The heat flux to the wall is also affected by the strength of the roll-up vortex ahead of the piston. These effects are both dependent of $v_p(t)$.

Third, note that in the course of piston motion the ignitable gas is located inside the test section closed on one side with the flat rigid wall (sealed flange) and on the other side with the flat surface of a moving piston. Despite the moving piston is sealed to test
section walls by O-rings some mass leakage \( m \) of the test gas to the buffer section through the gap inevitably exists. This effect is also dependent of \( v_p(t) \).

Thus, we come to the implication that different piston motion histories can also be a reason of the various inconsistencies in the measured ignition delays reported by different authors. Note that the local instantaneous piston velocity \( v_p(t) \) is hard to control experimentally because it is a function of different parameters and conditions (including \( m, m_0 \), etc.). Even if \( v_p(t) \) is somehow controlled or monitored, the mass leakage through piston rings is still hard to control.

For the sake of definiteness, we consider here the experiments with ignition of hydrogen–air mixture in an RCM reported in Leshevich and Penyazkov (2011). In the RCM experiments of Leshevich and Penyazkov (2011), the piston displacement \( \Delta t \) and the compression time \( t_c \) were interpreted as the main parameters relevant to ignition. Based on these parameters, one can readily obtain the average piston velocity \( \langle v_p \rangle = \Delta t/t_c \). The results of our numerical study reported below show that with an identical conditions (including \( \Delta t \)), the possibility to neglect frontal combustion comes from the fact that this combustion mode can arise only after localized self-ignition, which is the major object of the study. Moreover, even after the localized self-ignition combustion front propagation is too slow as compared with the apparent speed of spontaneous ignition waves traversing the precondensed mixture. The contributions from volumetric reactions \( \tau_V \) and \( Q_V \) were determined using the Particle Method (PM) (Frolov, Ivanov, Basara, & Sufa, 2013; Pope, 1985).

In the PM algorithm, the instantaneous local states of a turbulent reacting flow are presented as a set of interacting notional (Lagrangian) particles. Each ith particle has individual properties: the position in space \( x_i \), and three local instantaneous velocity components \( u_i(k = 1, 2, 3) \), volume \( V_i \), density \( \rho \), the static enthalpy \( h_i \), mass fractions of species \( y_i(l = 1, \ldots, N) \), and the statistical weight \( W_i \) used in determining the mean values of the variables over the ensemble of particles. For each ith particle, the following system of equations is solved, Pope, 1985:

\[
\rho \frac{Dx_i}{Dt} = u_i \\
\frac{D(\rho V_i)}{Dt} = \nabla f_i + f_{ih} \\
\rho \frac{Dh_i}{Dt} = \nabla q_i + \rho' \nabla q_i + D_{ij} + \rho \nabla (\frac{\partial h_i}{\partial x_j}) - (\frac{\partial h_i}{\partial x_j}) \nabla x_i
\]

where \( f_{ih} \) is the partial density of the ith species in the ith particle, \( f_{ih} \) is the change of the mass concentration of the ith species in the course of chemical reactions, \( P \) is the static pressure at the point of location of the ith particle, \( Q_V \) is the rate of energy release by chemical reactions in the ith particle, \( q_{ih} \) is the diffusion flux of the ith species to the ith particle, \( q_i \) is the momentum flux to the ith particle due to molecular viscosity, and \( q_i \) is the heat flux to the ith particle.

To determine the flux (exchange) terms in the PM, the classical model of linear decay to the mean is used, Pope, 1985:

\[
\nabla f_i = -0.5C (y_i - \bar{y_i}) \rho V_i \omega_i \\
(\rho')^{-1} \nabla (p' \cdot E - \tau') = -z_i (u_{ik} - U_{ik}) + A(t) \\
\nabla q_i = -0.5C (h_i - H_i) \rho \omega_i
\]

where \( C \approx 2.0 \) and \( \omega_i \approx 2.075 \) are coefficients; \( y_i, U_{ik}, H_i \) are the mean mass fraction of species \( i \), mean velocity, and mean enthalpy of the gas at the point of location of the ith particle, respectively; \( p' \) is the pulsating pressure component, \( \omega = \epsilon/k \) is the frequency of turbulent fluctuations; \( \tau' \) is the random function describing the influence of fluctuations of pressure and velocity on the motion of the particle; here, \( C_0 \approx 2.1, D(t) \) is a continuous random variable having normal distribution and satisfying the condition \( D(t) = 0 \) and \( D(t) = D(t) - \delta dt \) (\( \delta dt \) is the Kronecker symbol). The mean quantities \( y_i, U_{ik}, \) and \( H_i \) are determined either by interpolating the corresponding values of \( y_i, U_{ik}, \) and \( H \) (obtained from the solution of averaged Equations (1)–

\[
1560 \\
\]

\[
\]

2. Model

The three-dimensional (3D) motion of the gas inside the RCM test section, i.e., the time-dependent fields of velocity, pressure, density, temperature, and ignitable mixture species concentrations, is governed by Unsteady Reynolds Averaged Navier–Stokes (URANS), energy conservation, and species continuity equations:

\[
\rho \frac{DU_i}{Dt} = \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P_i}{\partial U_i} + \frac{\partial}{\partial x_j} \left( \frac{\partial E}{\partial x_j} - \rho U_i \right) \\
\frac{DP}{Dt} = \frac{1}{\rho} \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} \left( \frac{\partial P}{\partial x_j} \right) \\
\frac{DY_i}{Dt} = \frac{1}{\rho} \frac{\partial Y_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \frac{\partial Y_i}{\partial x_j} \right) - \rho' \frac{\partial q_i}{\partial x_j} + \rho_1 \frac{\partial q_i}{\partial x_j}
\]

where \( x_j (j = 1, 2, 3) \) is the coordinate; \( \rho \) is the mean density; \( P \) is the mean pressure; \( \mu \) is the dynamic viscosity; \( U_i \) is the mean velocity; \( \nabla \) is the fluctuating velocity component; \( \tau \) is the element of the viscous stress tensor; \( I = H + (1/2) \sum U_i^2 \) is the mean total enthalpy \( (H) \) is the mean static enthalpy \( \lambda \) is the thermal conductivity; \( T \) is the mean static temperature; \( \bar{y}_i (l = 1, \ldots, N) \) is the mean mass fraction of the ith species of the mixture \( N \) is the total number of species in the mixture); \( D_1 \) is the molecular diffusion coefficient of species \( i \); \( \bar{y}_i \) is the relative fraction of the mass fraction of ith species; and \( \delta \) are the mean source terms of mass and energy due to chemical reactions.

The turbulent fluxes of mass, momentum, and energy in Eqs. (1)–(3) are modeled using the standard \( k-\epsilon \) turbulence model (here, \( k \) is the kinetic energy of turbulence, and \( \epsilon \) is its dissipation).

In general, modeling of the chemical sources \( \tau_0 \) and \( Q \) for spontaneous ignition and turbulent combustion requires taking into account the contributions from both frontal combustion (index \( f \)) and volumetric reactions (index \( V \)):

\[
\tau_0 = \tau_f + \tau_V \]

\[
Q = Q_f + Q_V
\]

However, in view of the specific features of the phenomena described above, here we neglect the contribution of frontal combustion to the chemical sources assuming \( \tau_f = 0 \) and \( Q_f = 0 \). The possibility to neglect frontal combustion comes from the fact that this combustion mode can arise only after localized self-ignition, which is the major object of the study. Moreover, even after the localized self-ignition combustion front propagation is too slow as compared with the apparent speed of spontaneous ignition waves traversing the precondensed mixture. The contributions from volumetric reactions \( \tau_V \) and \( Q_V \) were determined using the Particle Method (PM) (Frolov, Ivanov, Basara, & Sufa, 2013; Pope, 1985).
(3) or by ensemble averaging over particles in a computational cell using the formulas

$$Y_i^l = \sum_i w_i^l \theta_i^l, \quad U_i^l = \sum_i w_i^l u_i^l, \quad H_i^l = \sum_i w_i^l h_i^l$$

(12)

where the statistical weight of the $i$th particle is given by

$$w_i^l = \rho_i^l V_i^l / \sum_i \rho_i^l V_i^l$$

(13)

System (1)–(3) in conjunction with the $k$–$\varepsilon$ turbulence model and the PM were solved by the caloric and thermal equations of state of an ideal gas with variable specific heat and supplemented by the initial and boundary conditions. All the thermophysical parameters of the gas were considered variable.

The calculation pressure field $P(x_0)$ and the local frequency of turbulent fluctuations $\omega$ required for solving the system of Equations (5)–(8) supplemented by additional relations (9)–(11), are determined by solving the averaged Equations (1)–(3) and the equations of the $k$–$\varepsilon$ turbulence model.

The most important advantage of the PM is the possibility of accurately determining the rates of chemical reactions in a turbulent flow: the source terms $f_{ih}$ and $Q_V$ are determined using the known mechanisms of chemical reactions as well as the instantaneous mass fractions $y_l^i (l = 1, \ldots, N)$ and temperature $T$ in the particle. The instantaneous local rate of change of the mass concentration of the $l$th species in the $i$th particle is calculated by the formula, Williams (1985):

$$J_{ih}^l = V_i^l W_i^l \sum_{k=1}^N (\rho_i^l \theta_i^l) A_k (\theta_i^l)^{n_k} \exp \left( - \frac{E_k}{R T_i^l} \right) \sum_{j=1}^N \left( \frac{\rho_j^l}{W_j^l} \right)^{n_j}$$

(14)

where $W_i^l$ is the molecular mass of the $l$th species; $\rho_i^l \theta_i^l$ and $\rho_i^l \theta_i^l$ are the stoichiometric coefficients for the $l$th species acting as a reagent or product in the $k$th reaction, respectively; $A_k$, $n_k$, and $E_k$ are the preexponential factor, the temperature exponent, and the activation energy for the $k$th reaction; $R$ is the universal gas constant; $L$ and $N$ are, respectively, the total numbers of reactions and species in the chemical mechanism.

The rate of energy release by chemical reactions in the $i$th particle is calculated by the formula, Williams (1985):

$$Q_V^i = \frac{1}{\rho_i^l} \sum_{k=1}^N H_k A_k (\theta_i^l)^{n_k} \exp \left( - \frac{E_k}{R T_i^l} \right) \sum_{j=1}^N \left( \frac{\rho_j^l}{W_j^l} \right)^{n_j}$$

(15)

where $H_k$ is the heat effect of the $k$th chemical reaction.

Knowing $J_{ih}^l$ and $Q_V^i$, one can determine the contribution of bulk reactions $\dot{r}_i$, and $Q_V^i$ to the chemical source terms $\dot{r}_i$ and $Q_V$:

$$\dot{r}_i = \sum_1^N w_i^l J_{ih}^l / \sum_1^N w_i^l, \quad Q_V = \sum_1^N w_i^l Q_V^i$$

(16)

The algorithm used for solving the governing equations is the combination of SIMPLE ("Semi-Implicit Pressure-Linked Equation") method of Patankar and Spalding (1972) with the semi-implicit Monte Carlo method for notional particles. For the solution of the governing Eqs. (1)–(3) a finite volume discretization and a 1st order-accurate implicit Euler time-stepping scheme is used. In order to accelerate the convergence of the SIMPLE method it incorporates the pressure–enthalpy coupling of Emans, Frolov, Lidskii, Posvyanskii, and Basara (2012) and Emans, Zunic, Basara, and Frolov, (2012). In this latter approach both the pressure correction and the enthalpy correction are calculated simultaneously in a common linear system such that not only the dependence of density on pressure is extrapolated, but also the dependence of pressure on enthalpy.

The mesh used consists of 100,000 hexahedral elements. A cross section along the cylinder axis is resolved by 50 cells along the axis and 60 cells perpendicular to the axis. The change of the geometry during the motion of the piston is accounted for by a uniform compression of the mesh in axial direction. The spacing in radial direction is nonuniform such that the region near the cylinder wall is resolved by an increased number of cells. The spacing in axial direction is uniform, but due to the compression it varies in time. After the compression has finished, the spacing in axial direction is 0.32 mm. The time stepping after the compression is uniform with a time step of 0.05 ms. As long as the piston moves, the time step is gradually reduced down to this value, starting with a time step of 0.25 ms. The Courant–Friedrich–Levi (CFL) number before the eventual ignition is always lower than 2.5, which indicates that the time stepping is well suited for the implicit procedure that is being used.

The chemical source terms are obtained using implicit numerical algorithm with internal time stepping to keep the CFL number here below 1. The combined algorithm has been thoroughly validated against experimental data on flame acceleration and deflagration-to-detonation transition in tubes with and without obstacles, Emans and Frolov (2011), as well as for shock-induced ignition and preflame autoignition in enclosures, Frolov, Emans, et al., 2013.

The CFD software platform used for the numerical solution is AVL FIRE 2011. The mentioned algorithm has been recently incorporated into it such that it can be used in a convenient way. The collocated discretization scheme employed in this study reflects the up-to-date standard of the computational technology; it has been explored in a number of preceding publications, starting with Demirdzic and Muzafarja (1995), and continuing with Ferziger and Peric (1996); Marthur and Murthy (1997); Basara (2004); and Basara, Alajbegovic, and Beader (2004).

3. Results

The fuel used was hydrogen. Only the stoichiometric hydrogen–air composition was considered in this particular study. For modeling hydrogen oxidation, a simplified single-step reaction mechanism was applied:

$$H_2 + H_2 + O_2 \rightarrow H_2O + H_2O$$

(17)

As reaction (17) is used only to calculate ignition delays in the RCM it is not that important that it does not account for water dissociation in the combustion products and other elementary reactions. The rate of hydrogen oxidation $[H_2]$ at elevated initial pressures $P$ (from 5 to 40 atm) and temperatures $T$ (from 850 to 1200 K) was calculated according to the simple relationship:

$$[H_2] = -8.0 \cdot 10^{11} P^{-1.15} [H_2]^2 [O_2] \cdot e^{-10000 \text{ (atm, mole, liter, s)}}$$

(18)

This relationship was obtained by fitting the ignition delays predicted by the validated detailed reaction mechanism of Basevich et al. (2007), Frolov, Ivanov, et al. (2013) and Frolov, Medvedev, Basevich, and Frolov (2013) with that provided by reaction (17). The comparison between ignition delays predicted by mechanism of Basevich et al. (2007), Frolov, Ivanov, et al. (2013) and Frolov,
Medvedev et al. (2013), reaction (17) and measurements for the stoichiometric hydrogen–air mixture at pressure 1 atm is given in Fig. 4. The corresponding experimental data are taken from Anagnostou, Brokaw, and Butler (1956) and Golovichev (1973).

For our examination, detailed experimental measurements of ignition delay times for the stoichiometric hydrogen–air mixture were made in the Luikov Institute for Heat and Mass Transfer. The RCM has been described in detail by Leshevich and Penyazkov (2011). The diameter of the RCM test section d was 50 mm. In the course of experiments, the following parameters were registered: the time history of the pressure in the test section $p(t)$, the compression time $t_c$, the piston displacement $\Delta l$. As discussed above, the two latter parameters allow one to obtain the average piston velocity $v_{pm}$, but the local instantaneous piston velocity $v_p(t)$ remains unknown.

For the calculations we have chosen 5 typical experimental test cases with different compression ratios $\beta$, different initial conditions in terms of $T_0$ and $p_0$, and different average piston velocity $v_{pm}$ (Table 1). The length $l_1$ and test section diameter $d$ were kept constant and equal to 16 mm and 50 mm, respectively. Test case #3 in Table 1 is the same as test case #1 but the computational mesh contains 800,000 rather than 100,000 cells. This mesh had in all directions of space and at all times half the cell width of our standard mesh. The calculation on this mesh was done in order to check if the proposed method is robust with regard to the spatial resolution.

In order to reproduce the experiment by numerical simulation, the appropriate boundary conditions have to be set. As was discussed above, in the experiment the test section is neither the adiabatic nor the closed system. Therefore some assumptions on heat transfer to the walls and mass leakage through the piston rings are needed to define boundary conditions for the calculations. In a preliminary study we have simulated the system with a constant piston velocity of $v_p(t) = v_{pm} = 6.26$ m/s at $T_0 = 292$ K, $p_0 = 12.86$ kPa, and $\beta = 22$ (test case #1 in Table 1). The curve with symbols in Fig. 5 shows the experimental pressure history for these conditions. Note that the experiment shows mixture ignition at these conditions (sharp pressure rise at $t \approx 57$ ms). To see how the computational model reproduces the experimental pressure curve in the RCM test section we have made three calculations with: (1) adiabatic walls and zero mass leakage $\bar{m} = 0$; (2) isothermal walls with $T_w = T_0 = 292$ K and $\bar{m} = 0$; and (3) isothermal walls with $T_w = T_0 = 292$ K and mass leakage $\bar{m} \neq 0$. In these calculations, the chemical reaction was purposefully deactivated to reproduce the pre-ignition stage of the experimental pressure curve.

Table 1

<table>
<thead>
<tr>
<th>Test case</th>
<th>$v_{pm}$, m/s</th>
<th>$T_0$, K</th>
<th>$p_0$, kPa</th>
<th>$\beta$</th>
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<tr>
<td>1</td>
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<td>292</td>
<td>12.86</td>
<td>22</td>
</tr>
<tr>
<td>2</td>
<td>5.34</td>
<td>292</td>
<td>12.86</td>
<td>22</td>
</tr>
<tr>
<td>3</td>
<td>6.26</td>
<td>292</td>
<td>12.86</td>
<td>22</td>
</tr>
<tr>
<td>4</td>
<td>6.36</td>
<td>292</td>
<td>11.50</td>
<td>24</td>
</tr>
<tr>
<td>5</td>
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<td>292</td>
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<td>6</td>
<td>7.01</td>
<td>292</td>
<td>11.50</td>
<td>24</td>
</tr>
</tbody>
</table>

The leakage mass flow $m$ is implemented as a normal-velocity boundary condition in the ring-shaped gap of 0.8 mm wide between the moving piston and the test section wall. Here the gas velocity (relative to the moving piston) is prescribed as $v_g = \sqrt{2\Delta p/(\rho \lambda)}$, where $\rho$ is the gas density, $\Delta p$ is the pressure difference between the interior of the test section, $p_1(t)$, and its exterior (atmospheric pressure $p_2$), and $\lambda = 0.49$ is the parameter that has been chosen such that the calculated pressure curve in Fig. 5 fits the experimental curve. This modeling is kept intentionally simple: it is inspired by the Bernoulli assumption that the pressure drop is proportional to the kinetic energy of the flow. Note that the value of parameter $\lambda$ was fixed in all calculations reported herein. In the future, this modeling will be improved.

As is seen from Fig. 5, the assumption on adiabatic or isothermal walls with $m = 0$ leads to a pressure at the end of piston motion that is significantly higher than in the experiment. Since the assumption of isothermal walls is a limiting case in the sense that the thermal inertia of the wall material is infinitely large, removing more energy from the test section is hard to justify. It is therefore reasonable to account for a certain leakage in the gap between the piston and the test section walls. The dotted curve in Fig. 4 indicates that the assumption of isothermal walls and $m \neq 0$ are sufficient to obtain the pressure curve which fits well with the experimental pressure history.

In the following, we focus on the same initial conditions as in Fig. 5, but with activated ignition chemistry and two different values of average piston velocity: $v_{pm} = 6.26$ m/s and $v_{pm} = 5.34$ m/s (test cases #1 and 2 in Table 1). Our calculations showed that the assumption $v_p(t) = v_{pm} = \text{const}$ does not allow predicting...
qualitatively the ignition behavior of the mixture, i.e., it is not possible to predict whether the reactive mixture spontaneously ignites or does not ignite at these conditions. For example, thick solid curves in Fig. 6 (marked $c = 0$) correspond to the assumption $v_p(t) = v_{pm} = 6.26$ m/s (Fig. 6a) and $v_p(t) = v_{pm} = 5.34$ m/s (Fig. 6b). As is seen, in the latter case the “no go” ignition behavior is predicted correctly by the calculation, but in the former case the calculation predicts “no go” whereas the experiment shows “go” ignition behavior (sharp pressure rise at $t \approx 57$ ms).

To demonstrate how the time history of piston velocity $v_p(t)$ affects the results of calculations (other conditions being equal, including $v_{pm} = \text{const}$), we formally represent $v_p(t)$ by power function $v_p(t) = a_c t^c$, where $a_c$ depends on $c$ and is chosen such that

$$
\int_0^t a_c t^c dt = v_{pm}
$$

The case $v_p(t) = v_{pm} = \text{const}$ discussed above corresponds to $c = 0$. Fig. 6a and b also show the results of calculations for $c = 1/8$, 1/2, and 1.0. Contrary to the case with $c = 0$ (no ignition) the cases with $0 < c < 1$ for the conditions of Fig. 6a predict ignition (sharp pressure rise). Moreover, the faster the piston speed at the end of compression (larger $c$) the shorter the ignition delay. As is seen from Fig. 6a, the best agreement between the calculations and the experiment in terms of the ignition delay is obtained at $c = 1$. Since we use here a simplified hydrogen oxidation reaction of Eq. (17) therefore there is not much sense here to speculate on the quantitative agreement between calculations and experiments. As a matter of fact, when addressing Fig. 6b, one sees that the calculations fit qualitatively with the experiment at $c = 0$ and 1/8 (no ignition) but fail to predict the “no go” ignition behavior at $c = 1/2$ and 1.0.

Now, let us find out the reason for the dependence of mixture ignition behavior on the time history of piston velocity, i.e., on the value of $c$. For this purpose, we have plotted Fig. 7 with the “trajectories” of the hottest states (particles) in the RCM test section (Fig. 7a), the mean temperature profiles along a certain line in the test section (Fig. 7b) and the hottest state (particle) temperature along the “trajectories” (Fig. 7c) for cases $c = 0$ (solid curves, no ignition predicted) and $c = 1/8$ (dashed curves, ignition predicted) in the conditions of test case #1. In the both computational runs, the hottest states (particles) in the flow field were identified at each time step by the maximum temperature $T_{\text{max}}$ starting from the end of compression ($t = t_c$). Since the particles are subject to renumbering, cloning and clustering in the computational algorithm, the location of the hottest state (particle) at each time step was mapped to a symmetry plane $z-r$ (“tube axis–tube radius”), thus presuming that the flow field exhibits axial symmetry. Remind that the left boundary of the plot in Fig. 7a ($z = 0$) corresponds to the closed end of the test section whereas the right boundary ($z = 16$ mm) corresponds to the piston surface at the end of compression stroke.

The particle “trajectories” in Fig. 7a are supplemented with time markers: the closed and open squares near the curves correspond to successive 1-ms time intervals for the cases with $c = 0$ and $c = 1/8$, respectively. Note that despite the curves in Fig. 7a were smoothed, the assumption on the axial flow symmetry seems to be well justified. The locations of the hottest states (particles) at the end of compression are shown by the corresponding arrows. Also, the ignition location in the case with $c = 1/8$ is shown by arrow.

It is seen from Fig. 7a that at the end of compression the hottest state (particle) is realized in both cases at the periphery of the roll-up vortex close to the side wall of the test section at $r \approx 22.5$ mm. In the case with $c = 1/8$ the hottest point is located at a somewhat larger distance from the piston ($z \approx 5$ mm) than in the case with $c = 0$ ($z \approx 7.5$ mm). It is interesting that despite different piston velocities at the end of compression the hottest states in both cases follow approximately the same “trajectory”, but the time at which they pass a certain point at the $z-r$ plane is not the same. With time, the hottest state moves first towards the piston surface and then moves in the opposite direction drifting closer to the test section center-line. Spontaneous ignition (at $c = 1/8$) occurs locally at $z = 5$ mm and $r \approx 10$ mm. As for the hottest state (particle) in the case with $c = 0$ and no ignition, it moves towards the vortex center with the “trajectory” resembling Archimedean spiral.

Fig. 6b shows the mean temperature profile in the test section along the line parallel to the z-axis through the radial position $r = 22.5$ mm — the position where the hottest state is realized at $t = t_c$, i.e., at the instant when piston stops. One can see that the temperature in the case with $c = 1/8$ is higher by several degrees.

Fig. 7b contains also the temperature profiles of the same calculations with $c = 0$ and $c = 1/8$ on a finer mesh of test case #3. The time stepping in these calculations was the same as on our standard mesh. In fact, the plotted temperature profiles show that the predicted temperatures near the region of the hottest state (particle) are indeed close to the ones predicted with the coarser mesh. Moreover, the qualitative behavior (no ignition for $c = 0$ and ignition for $c = 1/8$) is also predicted if the finer mesh is used.
Fig. 7c shows the time histories of the temperature in the hottest particles at $c = 1/8$ and $c = 0$ indicating that the slightly higher initial (at $t = t_c \approx 53.2$ ms) temperature in the former case ($T_{\text{max}} \approx 904$ K) results in ignition whereas in the latter case ($T_{\text{max}} \approx 900$ K) ignition fails.

To further illustrate the differences between the cases with $c = 1/8$ and $c = 0$ consider Figs. 8 and 9. Shown in these figures are the predicted temperature (Fig. 8) and velocity (Fig. 9) fields plotted as slices through the test section axis for different time instants at $t \geq t_c$ for the conditions of test case #1. For the sake of comparison, the figures contain both cases with the upper part corresponding to the case with $c = 0$ (no ignition) and the lower part to the case with $c = 1/8$ (ignition). The parts are mirrored with respect to the test section axis, so that the upper and lower boundaries correspond to the side wall of the test section, the left boundary corresponds to the closed end of the test section, and the right boundary corresponds to the piston surface. Squares at each snapshot indicate the instantaneous position of the hottest state in the flow. It is seen from Fig. 8 that the temperature differences between the hottest states in both cases are small compared to the temperature differences in the entire flow field. As for the velocity fields, they are different only during $\approx 2$ ms after the end of compression and then these fields appear to be very similar to each other. Thus, from observing the flow field alone one might be tempted not to discern the differences between both cases that are responsible for the qualitatively different behavior of the system.

Finally, let us consider test cases #4 to 6 in Table 1. These test cases have the same compression ratio $\beta = 24$, initial pressure $p_0 = 11.50$ kPa, and initial temperature $T_0 = 292$ K but different average piston velocities: $v_{\text{pm}} = 6.26, 6.35$ and $7.01$ m/s. Fig. 10 compares the experimental pressure curves for these test cases with the calculated pressure curves corresponding to different values of parameter $c$ in the piston velocity law $v_p(t) = a_0 t^c$. Clearly, the calculations with different $c$ values correlate qualitatively with the experiments. As for the quantitative comparison, the condition $c = 0$ seems to be the most appropriate.

4. Concluding remarks

This study unambiguously indicates that the time history of piston motion in an RCM affects the final state of a test mixture at the end of compression stroke and therefore influences the phenomena relevant to test mixture ignition. This conclusion is made based on the simulation of RCM operation using a coupled 3D URANS – PM algorithm capable of catching turbulence–chemistry interaction. More specifically, the calculations show that different laws of piston motion at a fixed average piston velocity (i.e., fixed piston displacement and fixed compression time) and fixed compression ratio result in different evolution of mean pressure, temperature and velocity fields in the RCM test section leading to different ignition behavior. The reasons for the arising differences lie in the fact that the local instantaneous piston velocity determines the roll-up vortex structure, strength and turbulence dissipation in it, heat transfer in test-section walls, and mass leakage through piston rings.

Fig. 7. (a) “Trajectories” of the hottest state (particle) after the end of compression mapped to a symmetry plane (symbols mark 1-ms time interval) in test case #1; (b) temperature profiles at $r = 22.5$ mm (position of the hottest particles at the end of the compression); and (c) time histories of temperature along the “trajectories” of the hottest states (particles): thick solid curves and closed squares correspond to $c = 0$, thick dashed curves and open squares correspond to $c = 1/8$; thin solid and dashed curves in Fig. 7b correspond to $c = 0$ and 1/8, respectively, in test case #3 with a finer mesh.
Fig. 8. Calculated temperature fields (degrees Kelvin) in the RCM test section at $t = 53.2$ ms (end of compression), $t = 55.2$ ms, $t = 57.2$ ms, and $t = 59.2$ ms (from left to right), upper part: $c = 0$ (no ignition), lower part $c = 1/8$ (ignition), test case #1.
Fig. 9. Calculated fields of the velocity vector length (meters per second) in the RCM test section at $t = 53.2$ ms (end of compression), $t = 55.2$ ms, $t = 57.2$ ms, and $t = 59.2$ ms (from left to right), upper part: $c = 0$ (no ignition), lower part $c = 1/8$ (ignition), test case #1.
be explained, at least partly, by different time histories of piston motion in different machines and even in the same RCM due to cycle-to-cycle variations in the piston velocity history.

As a matter of fact, there is a need in the development of a sort of standard RCM — the analog of a standard 20-L closed-bomb test apparatus of American Society for Testing and Materials (ASTM). Such a standard RCM could be used for collecting data on low-temperature ignition characteristics of ignitable mixtures and for validating various reaction mechanisms. It goes without saying that standardization of measuring tools implies deep understanding of all accompanying physical and chemical phenomena. Therefore further fundamental computational and experimental studies are required.

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