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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.

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; Gersen, 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

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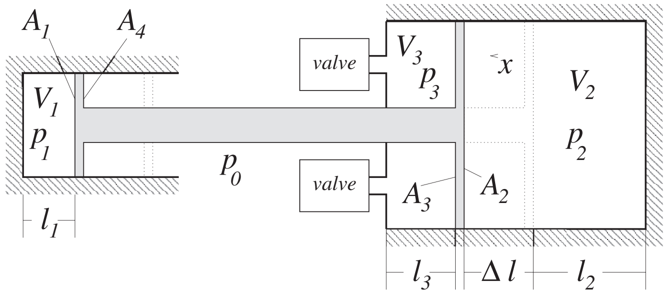


Fig. 1. Schematic of the Rapid Compression Machine with a piston assembly.

test gas undergoes compression accompanied with pressure, temperature and density increase. After a preset displacement Δl (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_{ign}.

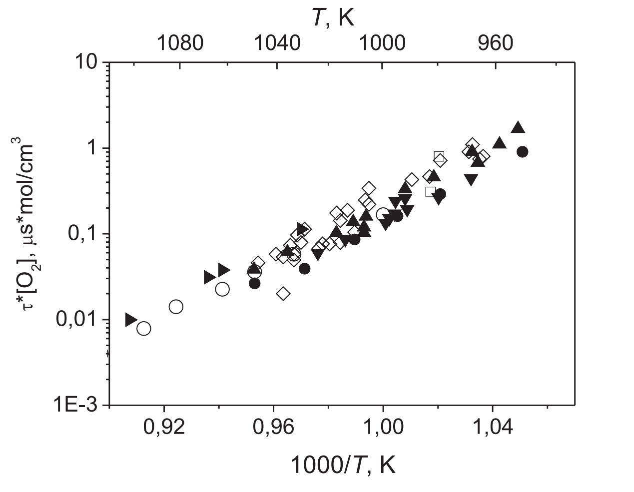
The ignition event in the test section is usually registered applying various optical and pressure-sensing techniques. To better identify the ignition conditions in terms of instantaneous pressure p_1 and temperature T_1, ignition in the standard procedure is required to occur after the piston stops. 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 $\tau_{ign} = t_{ign} - t_c$.

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 τ_{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 τ_{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 of the piston velocity evolution, i.e., 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.



	Ref	Mixture	Pressure
□	Leshevich & Penyazkov (2011)	$H_2/O_2/N_2$ – 2/1/3.76	31.85 atm
◊	Lee & Hochgreb (1998)	$H_2/O_2/Ar$ – 2/1/5	6–40 atm
○	Mittal et al. (2006)	$H_2/O_2/N_2/Ar$ – 2/1/7/4.5	33.6 atm
●	Mittal et al. (2006)	$H_2/O_2/N_2/Ar$ – 2/1/15/82	33.55 atm
▶	Mittal et al. (2006)	$H_2/O_2/N_2/Ar$ – 2/1/2.9/10.1	29.6 atm
▲	Gersen et al. (2008)	$H_2/O_2/Ar$ – 2/1/5	16–21 bar
▼	Gersen et al. (2008)	$H_2/O_2/Ar$ – 2/1/5	20–52 bar

Fig. 2. Ignition delay vs. temperature for hydrogen containing mixtures: experimental points from Lee and Hochgreb (1998); Mittal et al. (2006); Gersen et al. (2008); Leshevich and Penyazkov (2011).

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

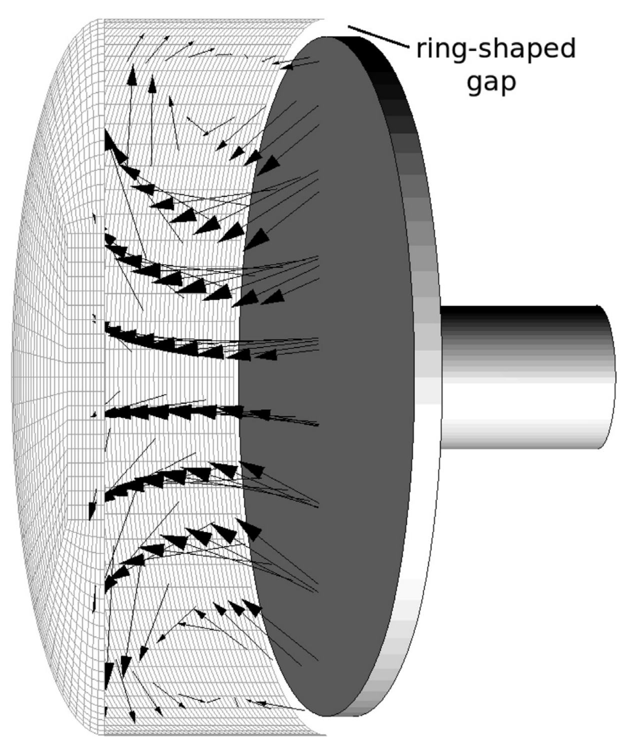


Fig. 3. Roll-up vortex ahead of the piston with streamlines and velocity vectors.