Aerodynamics inside a rapid compression machine

Gaurav Mittal, Chih-Jen Sung *

Department of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland, OH 44106, USA

Received 9 May 2005; received in revised form 11 October 2005; accepted 22 October 2005

Available online 15 December 2005

Abstract

The aerodynamics inside a rapid compression machine after the end of compression is investigated using planar laser-induced fluorescence (PLIF) of acetone. To study the effect of reaction chamber configuration on the resulting aerodynamics and temperature field, experiments are conducted and compared using a creviced piston and a flat piston under varying conditions. Results show that the flat piston design leads to significant mixing of the cold vortex with the hot core region, which causes alternate hot and cold regions inside the combustion chamber. At higher pressures, the effect of the vortex is reduced. The creviced piston head configuration is demonstrated to result in drastic reduction of the effect of the vortex. Experimental conditions are also simulated using the Star-CD computational fluid dynamics package. Computed results closely match with experimental observation. Numerical results indicate that with a flat piston design, gas velocity after compression is very high and the core region shrinks quickly due to rapid entrainment of cold gases. Whereas, for a creviced piston head design, gas velocity after compression is significantly lower and the core region remains unaffected for a long duration. As a consequence, for the flat piston, adiabatic core assumption can significantly overpredict the maximum temperature after the end of compression. For the creviced piston, the adiabatic core assumption is found to be valid even up to 100 ms after compression. This work therefore experimentally and numerically substantiates the importance of piston head design for achieving a homogeneous core region inside a rapid compression machine.

© 2005 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Keywords: Rapid compression machine; PLIF of acetone; Adiabatic core hypothesis; Computational fluid dynamics; Autoignition

1. Introduction

In a rapid compression machine (RCM) study, primary experimental data consist of the pressure trace of a given reacting mixture. A typical pressure trace before autoignition taking place shows a rapid rise in pressure during the compression stroke, which is of the order of 15–40 ms, followed by a gradual decrease in pressure due to heat loss from a constant-volume chamber at the end of compression. Although in principle RCM simulates a single compression event, complex aerodynamic features can affect the state of the reacting core in the reaction chamber. Previous studies (e.g., [1–3]) have shown that the motion of the piston creates a roll-up vortex, which results in mixing of the cold gas pockets from the boundary layer with the hot gases in the core region. Such undesired mixing leads to difficulties in accurately characterizing the state of the reacting mixture.

In modeling the RCM experiments, for simplicity it is often assumed that the aerodynamic effects do not play any significant role at the short time scales...
encountered in the RCM. It is further assumed that the core gas, away from the thermal boundary layer, is compressed adiabatically. Thus, temperature evolution is determined from the measured pressure profile by assuming the adiabatic core hypothesis. Based on this hypothesis, the core temperature at any instant during compression, $T(t)$, can be determined from the experimentally measured pressure, $P(t)$, according to the relation $\int_{T_0}^{T(t)} \frac{\gamma}{\gamma-1} \frac{dT}{T} = \ln\left[\frac{P(t)}{P_0}\right]$, where $P_0$ is the initial pressure, $T_0$ the initial temperature, and $\gamma$ the specific heat ratio. Furthermore, to model the RCM data, the computed pressure variation needs to match with the experimental pressure trace by including an empirically determined heat transfer coefficient or volume expansion with a zero-dimensional model [4–6]. However, substantial discrepancies have been observed between data taken from different rapid compression machines even under similar conditions of temperature and pressure [7,8]. These discrepancies are attributed partly to the different heat loss characteristics after the end of the compression stroke and partly to the difference in aerodynamics between various machines.

The effect of aerodynamics is particularly more complicated because it does not show up in the pressure trace and it may lead to significant temperature gradients and ultimately to the failure of the adiabatic core hypothesis. If the aerodynamic effect becomes significant and the adiabatic core hypothesis fails, there is no easy way to determine the temperature inside the reaction chamber. As a result, unambiguous determination of the state of the reacting mixture and systematic characterization of the resulting aerodynamic field inside an RCM are important for obtaining reliable kinetic data from RCMs and bridging the gap between data taken from different machines.

Several studies have contributed to the understanding of the aerodynamics and temperature field inside an RCM by computational fluid dynamics (CFD) calculations and experimental measurements. Griffiths et al. [1] numerically showed that the hot core region generated at the end of compression is virtually adiabatic and spans approximately 70% of the volume of the combustion chamber at the end of compression. Griffiths et al. [1] also observed differences between computational results using spatially uniform conditions and CFD simulation. Differences between two sets of computations were attributed to the effect of temperature gradient that was accounted for in CFD analysis [1]. In the recent study of Clarkson et al. [2], the temperature field was imaged by Rayleigh scattering and laser-induced fluorescence (LIF) of acetone. Acetone-LIF was found to nicely characterize the temperature variations in the RCM, whereas Rayleigh scattering was relatively less sensitive [2]. It was experimentally observed that the roll-up vortex had penetrated the center of the combustion chamber at the end of compression [2]. The temperature difference between the hot gases and the roll-up vortex was estimated to be 50 K [2]. Furthermore, LIF of acetone generated by decomposition of di-$t$-butyl peroxy unambiguously showed the temperature stratification at the center of the reaction chamber [2].

Griffiths et al. [9] investigated temperature and concentration fields in a rapid compression machine by using a number of experimental techniques, including Schlieren photography, planar laser-induced fluorescence (PLIF) of acetone, PLIF of formaldehyde, and chemiluminescence imaging. In order to illustrate the interaction of chemistry with the temperature field in the RCM, Griffiths et al. [9] contrasted the combustion behavior of di-$t$-butyl peroxy with that of $n$-pentane. The overall reaction of the former is characteristic of thermal ignition, while the combustion of the latter was investigated in the compressed temperature range exhibiting a negative temperature dependence of the overall reaction rate. With imaging being taken up to 10 ms after the end of compression, results showed that the di-$t$-butyl peroxy reaction proceeded faster in the zone of peak temperature [9]. Somewhat similar behavior was observed for $n$-pentane combustion when the compressed temperature was at the lower end of the negative temperature dependence range [9]. By contrast, at compressed temperatures close to the upper end of the negative temperature dependence region, the reaction in the cooler zone developed faster and the temperature inhomogeneity inside the reaction chamber rapidly smoothed out [9]. However, Griffiths et al. [9] pointed out that spatial inhomogeneity of concentrations of intermediates can be there, which would affect the eventual evolution of spontaneous ignition.

Griffiths et al. [10] used chemiluminescence imaging along with filtered Rayleigh scattering in a rapid compression machine to characterize the transition from nonknocking to knocking reaction and the evolution of the spatial development of the reactivity. Results from filtered Rayleigh scattering gave evidence of a cooler core region at compressed temperatures below the negative temperature dependence region [10]. In contrast, Rayleigh scattering did not show a cooler core at compressed temperatures within the region of negative temperature dependence. Hence, the effect of the negative temperature dependence of reaction rate is to smooth out the temperature inhomogeneity inside the reaction chamber [10].

Lee and Hochgreb [3] theoretically demonstrated that the roll-up vortex due to the piston motion can be counteracted by deliberately machining a crevice into the side of the piston. Creviced piston allowed more accurate predictions of the reacting temperature from
pressure–time records. Predictions of a simple heat transfer model in conjunction with a creviced piston were found to agree well with experimental pressure history [3].

Desgroux et al. [11,12] made direct measurements of temperature in an RCM using thermocouple and single point Rayleigh scattering. These measurements confirmed the existence of an adiabatic core gas at the end of compression. Rayleigh scattering measurements were made with a temperature accuracy of 3–4%, but after the end of compression the local temperature exhibited a standard deviation of 10–15% [11]. Desgroux et al. [12] conducted fine-wire thermocouple measurements for nonreactive and reactive mixtures at different radial locations. They observed a uniform temperature field for a few milliseconds after the end of compression and subsequent development of temperature inhomogeneity due to heat loss to the wall and gas recirculation [12]. For nonreactive mixtures the temperature inhomogeneity persisted after compression, whereas for reactive iso-octane mixtures a temperature-leveling effect, ascribed to the negative temperature coefficient of reaction rate, was observed [12].

Donovan et al. [13] took direct thermocouple measurements in a free-piston rapid compression facility to assess the adiabatic core hypothesis. Measurements were corrected for slower response of the thermocouple. Donovan et al. [13] asserted that experimental measurements at the end of the compression stroke justified the adiabatic core gas assumption. However, the thermocouple measurements failed to give a true representation of temperature after the end of compression because of the failure of the model used to correct the time response of the thermocouple [13].

Recently, Würmel and Simmie [14] conducted CFD studies of a twin-piston rapid compression machine using Star-CD. From the CFD simulations, the piston head crevices were optimized for the twin-piston RCM in terms of volume, location, and the dimension and geometry of the channel connecting the crevice and the chamber. The channel connecting the crevice and the chamber was optimized and the ideal geometry was found to be rectangular [14]. An angled channel design was seen to help somewhat in the cooling of the trapped gas in the piston head crevice. Würmel and Simmie [14] also observed strong dependence of the crevice performance on the test gas used. Specifically, although an optimal crevice was identified for test gases such as nitrogen, oxygen, and argon, it was not possible when using helium, due to the associated high heat loss. Instead of helium, the use of xenon as a bath gas for RCM experiments was recommended [14].

The present investigation aims to extend the previous efforts by experimentally and numerically studying the effect of the piston head geometry on aerodynamics and temperature field inside an RCM. It has implications for kinetic modeling in the sense that how well the prediction of the adiabatic core hypothesis matches with the actual temperature in the reaction chamber for a long time duration after the end of compression. Requirement of experimental data, particularly under the conditions of homogeneous charge compression ignition (HCCI) operation, requires the ability to sustain unambiguous reaction conditions for longer times. This is so because the relevant HCCI conditions are extremely lean or highly diluted, which significantly increases the ignition delay times. Therefore, it is particularly important to characterize the state of the aerodynamics and the resultant temperature field for long time duration after the end of compression stroke.

In the present work, temperature field inside an RCM is studied using planar laser-induced fluorescence (PLIF) of acetone. Laser diagnostic technique in an RCM offers many advantages in comparison to the thermocouple measurements. Thermocouple measurements suffer from the drawback that one cannot readily obtain information about instantaneous spatial variation of temperature. Moreover, there will be aerodynamic disturbances if the thermocouple probe is not sufficiently fine [12]. Additionally, correction of the measured temperature due to the slow time response of the thermocouple requires knowledge of the velocity field inside the chamber. The validity of the model used to determine the velocity field and correct for time response may be under question. By resorting to a longer compression time, as conducted in [12], while the effect of thermal inertia of the thermocouple can be minimized, aerodynamics at long compression times may not be a true representation of what happens at short compression times. In contrast, temperature mapping using the laser techniques is practically nonintrusive and is capable of giving instantaneous spatially resolved temperature field.

Both a flat piston and a creviced piston are employed and compared in the present study. These experiments will demonstrate whether the uniformity of the temperature field is indeed improved by using a creviced piston, as suggested by the earlier theoretical study [3]. The present investigation is particularly useful because experiments are conducted on the same RCM. The mapping of the temperature field is carried out for two different piston head configurations under varying operating conditions for a long time duration after the compression. In order to investigate the effect of the piston geometry on ignition delay, experiments are also conducted for autoignition of iso-octane using both piston head configurations. In addition, numerical simulations are carried out using Star-CD CFD package. Computed results
further provide insights into the nature of the aerodynamics inside an RCM. Based on these experimental and computational studies, conditions under which the adiabatic core hypothesis can be satisfactorily applied are delineated.

In the following sections we will first highlight the features of the RCM employed herein. Experimental specifics for the ignition delay measurements and PLIF of acetone are then described, followed by experimental and numerical results on the characterization of aerodynamics inside the RCM.

2. Experimental

2.1. Rapid compression machine

Fig. 1 shows the schematic of the present RCM system that consists of a driver piston, reactor piston, hydraulic motion control chamber, and a driving air tank. The driver cylinder has a bore of 5 in. (12.7 cm) and that of the reactor cylinder is 2 in. (5.08 cm). The machine is pneumatically driven and hydraulically stopped. Stroke can be varied between 7 and 10 in. (17.78 and 25.4 cm) by adjusting the spacers on the hydraulic cylinder. Clearance is also adjustable and can be varied by using split shims between the hydraulic cylinder head and the reactor cylinder. Further details of the present rapid compression machine can be found in [15]. The cylindrical reaction chamber is equipped with the sensing devices for pressure and temperature, gas inlet/outlet ports for preparing the reactant mixture, and quartz windows for optical access. Dynamic pressure during compression is measured using Kistler 6125B transducer with a 5010B charge amplifier.

In order to study the effect of the piston head design on aerodynamics in an RCM, experiments are conducted for two different piston head configurations: a creviced piston and a simulated flat piston. An enlarged view of the configuration of the creviced piston head is also shown in Fig. 1. The location of the crevice is on the cylindrical surface of the piston and the piston face is kept flat. On the other hand, the term “flat piston” indicates a piston that does not have a crevice along its cylindrical periphery and hence is flat on the face and along the piston circumference. In the present study, the flat piston head is simulated by filling the crevice volume with a pack of o-rings. This filling results in approximately 90% reduction in the crevice volume and gives an almost flat piston.

Two sets of experiments are conducted and compared using both piston head configurations. First, ignition delays for stoichiometric iso-octane/oxygen/inert gas mixtures are measured in the temperature range of 684 to 878 K, from which the effect of piston...
head configuration on autoignition is demonstrated. Second, PLIF imaging of acetone for temperature field mapping is carried out under conditions of relatively low pressure (approximately 12 bar) and high pressure (approximately 39.5 bar). These experiments also provide insights into the effect of pressure on the resulting temperature field inside the rapid compression machine.

2.2. PLIF of acetone

For the characterization of the temperature field, laser-induced fluorescence of acetone tracer in nitrogen is studied from the end of the compression stroke. The mixture consists of 1 to 2% (by concentration) acetone and remaining nitrogen. The schematic of the PLIF imaging setup is also depicted in Fig. 1. An approximately 5-mm-wide laser sheet with a waist of 50 µm is made to traverse the central plane of the combustion chamber, which is equidistant from the reactor piston face and the end of the chamber. The combustion chamber is equipped with two 0.66-in. (1.67-cm) diameter optically flat quartz windows for the traversal of the laser sheet. The end of the chamber is fitted with a 2-in. (5.08-cm) diameter and 1.7-in. (4.318-cm) thick quartz window, which provides full view of the combustion chamber for fluorescence imaging. An intensified CCD camera (Princeton Instruments, PI-MAX, 1024 × 256 pixels) with a UV lens (Nikon, f = 105 mm) is placed perpendicular to the laser sheet in order to record the fluorescence images. A WG305 (Schott) filter is used to filter scattered light from the fluorescence signal. A frequency-doubled Continuum Nd:YAG system is used in conjunction with a dye laser filled with Rhodamine 590 solution. The resulting laser energy at wavelength of 279 nm is around 8 mJ/pulse.

The synchronization of the laser firing with machine is achieved in the following manner. The laser is continuously fired at a repetition rate of 10 Hz. The signal generated from the start of the ICCD camera acquisition is used to actuate a relay after a specified time delay. Actuation of the relay fires the RCM. A subsequent laser pulse, which occurs after the end of compression, provides the pumping source for the induced fluorescence. The timings of laser pulses and pressure trace of RCM are simultaneously recorded using a data acquisition system, which allows accurate determination of the timing of laser pulse relative to the end of compression. After every experiment, the laser optics is realigned to correct for any minor movement of the machine as a result of firing. Since the repetition rate of the laser system is 10 Hz, PLIF images are single-shot measurements.

![Fig. 2. Ignition delay time versus the adiabatic core temperature at TDC for stoichiometric iso-octane/oxygen/inert mixtures. Composition: C8H18/O2/inert = 1/12.5/47. Initial conditions: P0 = 331 Torr and T0 = 297 K. The adiabatic core temperature at TDC is varied by changing the composition of the inert gases.](image)

3. Experimental results

3.1. Ignition delay

Experiments are generally conducted for a stroke of 10 in. (25.4 cm) and clearance of 0.525 in. (1.33 cm). Time for the compression stroke is approximately 30 ms, and the geometric compression ratio when using a creviced piston is 15.1. Fig. 2 shows a plot of ignition delay, measured in the present RCM, versus the adiabatic core temperature at the top dead center (TDC), Tc, for stoichiometric iso-octane/oxygen/inert gas mixtures. Based on the experimental pressure trace, Tc is calculated according to $\frac{1}{T_0} \int_0^T \frac{dP}{T} = \ln \left( \frac{P_c}{P_0} \right)$, where $P_c$ is the compressed pressure at TDC. Experiments are conducted using a flat piston and a creviced piston. For a given piston head configuration, the adiabatic core temperature is varied by changing the composition of the inert gases (argon and nitrogen), while keeping a fixed compression ratio. Results of the present work are also compared with the experimental data of Minetti et al. [16] under similar conditions of pressure, composition, and equivalence ratio. For the creviced piston, the initial pressure and the initial temperature are kept fixed at 331 Torr and 297 K, respectively. For the flat piston, clearance is increased to compensate for the absence of the crevice so that the conditions at TDC are identical to those for the creviced piston when same initial conditions of pressure, temperature, and composition are used. This results in adiabatic core temperature at TDC ranging from 684 to 878 K and pressure at TDC varying from 13.3 to 16.25 bar.

In spite of similar conditions, Fig. 2 demonstrates substantial discrepancies among different sets of experimental data. This comparison shows that not only the data from different RCMs under similar test con-
ditions may be different, but also for the same RCM there may be significant differences depending upon the configuration of the piston head and the final reacting volume. Furthermore, it is seen from Fig. 2 that when a flat piston is used, ignition delays are significantly reduced as compared to those obtained by using a creviced piston. It is therefore expected that changing from a creviced piston head to a flat piston head significantly affects the heat loss and the resulting aerodynamics inside the RCM, and the effect reflects in the form of considerable change in ignition delay. This example is presented here to highlight the importance of the piston head configuration effect on ignition delay.

3.2. Acetone fluorescence

The acetone fluorescence signal can be highly sensitive to temperature. At 279 nm excitation, fluorescence signal reduces by 42% as temperature increases from 600 to 800 K [17,18]. Fig. 3 shows a representative single-shot PLIF image of a homogeneous acetone/nitrogen mixture at room temperature of 297 K and pressure of 44 bar, along with the associated photon count integrated along the width of the laser sheet. For this experiment, a mixture of acetone and nitrogen at an initial pressure of 2.91 bar is gradually compressed by slowly moving the reactor piston. Such compression is nearly isothermal because the compressed gases are allowed to cool down to the room temperature. After the desired compressed pressure is reached, the fluorescence measurement is subsequently taken. Laser sheet enters from the right side of the image. The location of cylinder wall is also shown in the figure. Decay in the fluorescence signal from right to left is because of strong absorption. According to the Beer–Lambert law, in a homogeneous field with uniform temperature and concentration, signal decays exponentially due to absorption of the laser intensity. By correcting for absorption and incorporating for temperature sensitivity of fluorescence signal, it is possible to determine the resultant temperature field from fluorescence signal. Parameters for temperature sensitivity of acetone fluorescence are taken from Thurber et al. [17,18].

Using the fluorescence intensity shown in Fig. 3, Fig. 4 demonstrates the procedure for deducing the temperature distribution. In Fig. 4, radial direction equal to 0 corresponds to the central axis of the cylindrical chamber, while 2.54 and −2.54 cm represent the cylinder wall on either side. Moreover, the dotted line is the actual fluorescence signal, while the dashed line represents the exponential decay in the fluorescence intensity, as calculated using the Beer–Lambert law and the known temperature of 297 K. In addition, the deduced temperature distribution is denoted by the solid line. It is seen from Fig. 4 that in a uniform temperature field, signal follows the exponential decay feature and the deduced temperature nicely predicts the temperature distribution. In Fig. 4, the deduced temperature is noted to be within ±4 K, which is within 1.35% of the actual temperature. This gives an estimate of the uncertainty of the deduced temperature due to the noise in the fluorescence signal.

When there exists temperature nonuniformity in the chamber, knowledge of the temperature at one anchor point is required to deduce the temperature distribution from the fluorescence signal. Relative to this anchor point, temperature along the radial direction can subsequently be deduced by knowing the temperature dependence of the fluorescence intensity.

![Fig. 3. A representative single-shot acetone-PLIF image and the associated photon counts integrated along the width of the laser sheet. Chamber conditions: pressure = 44 bar and temperature = 297 K. Laser sheet enters from the right side of the image.](image3)

![Fig. 4. Temperatures deduced from the fluorescence signal. Chamber conditions: pressure = 44 bar and temperature = 297 K. Dotted line: raw fluorescence intensity. Dashed line: calculated fluorescence intensity using the Beer–Lambert law. Solid line: deduced temperature distribution.](image4)
However, such an anchor temperature is difficult to be measured during the actual RCM experiment. In the present work, the maximum temperature in the chamber at any time instant is taken as the adiabatic core temperature, calculated from the pressure trace based on the expression \[ \int_0^{T(i)} \frac{\gamma}{\gamma - 1} \frac{dT}{T} = \ln \left( \frac{P(t)}{P_0} \right) \].

The procedure to deduce the temperature distribution from the integrated fluorescence intensity profile is as follows. An anchor point in the fluorescence intensity profile is first arbitrarily chosen at some pixel inside the chamber and given a temperature value equal to the adiabatic core temperature derived from the experimental pressure trace at that instant. Subsequently, the temperatures at other radial locations are determined by marching radially in both directions toward the wall from this anchor point. While marching radially, correction for absorption is conducted according to the Beer–Lambert law. According to this law, attenuation in the laser intensity \( I \) as the laser traverses a length \( dx \) is expressed as \( I/I_0 = \exp(-\sigma n dx) \), where \( I_0 \) is the incident laser intensity, \( \sigma \) is the absorption coefficient, and \( n \) represents the acetone number density. At each marching step, after correcting for the absorption, the temperature is calculated from the knowledge of the temperature dependence of the fluorescence intensity, for which data is taken from Thurber et al. [17,18]. By marching radially from the first chosen anchor point, the temperature distribution along the entire domain of the chamber is therefore deduced. If the resulting maximum temperature in the chamber is higher than the adiabatic core temperature, the temperature of the anchor point is reduced for the next iteration. The iteration procedure continues until the maximum deduced temperature in the chamber equals the adiabatic core temperature.

It has to be pointed out that the assumption of the maximum temperature being equal to the adiabatic core temperature does not affect the pattern of the deduced temperature in any way. If the actual maximum temperature is somewhat lower than the adiabatic core temperature, the entire temperature profile would shift downward, without affecting the pattern of the temperature distribution.

3.3. Flat piston

3.3.1. Low compressed gas pressure

Fig. 5 shows the experimental results conducted at an initial pressure of 236 Torr and an initial temperature of 297 K using the simulated flat piston. The mixture consists of 2% acetone in nitrogen. At the end of compression, the gas pressure and temperature are 12.5 bar and 780 K, respectively. Again, the raw fluorescence signal is shown as the dotted line and the deduced temperature is denoted as the solid line. Exponential decay of the fluorescence intensity, as may be observed in a uniform temperature field, is shown as the dashed line. Time 0 is taken as the end of the compression stroke. The fluorescence signal at 1 ms after compression shows increased intensity in the central portion of the chamber. Any deviation of fluorescence signal from exponential decay is indicative of temperature inhomogeneity. In addition, any hump corresponds to reduced temperature, while any depression indicates an increase in the temperature. At 1 ms, an increased fluorescence intensity in the central portion is due to the effect of the roll-up vortex, which brings in cold gases from the boundary layer to the center of the chamber. In the temperature field, this increase in fluorescence intensity corresponds to approximately 100 K reduction in the temperature. At 6 ms postcompression, as we go from the wall to the centerline, there are alternating cold and hot regions. Apart from the temperature reduction of approximately 50 K in the central regime, there is another zone of low temperature near the wall. The reason for this type of temperature nonuniformity will be discussed later on along with the discussion of computational results.

At time steps of 8 and 18 ms, the width of the central depression zone increases due to thermal transport, whereas the temperature difference associated with this depression decreases. In addition, the effect of the side depression becomes more pronounced. Similar features are observed in the temperature field at subsequent time steps. Even at a long time scale of 129 ms, sharp temperature gradients exist in the chamber. Furthermore, these PLIF results are consistent with those of previous studies [2,9].

Since only one PLIF measurement can be imaged during every run of the RCM, aerodynamic features captured at the specified time instance may vary slightly in different runs. For instance, at 19 ms in Fig. 5, instead of depression in the temperature distribution at the center, a peak in the center and two adjacent zones of low temperature are observed. This would suggest that the cold gases flowing across the piston head did not reach the center of the chamber from either direction. Although slightly different pattern may be observed in different runs even at the same reference time after compression, it does not alter the conclusion that the use of the flat piston leads to substantial temperature nonuniformity due to the effect of the roll-up vortex. In general, PLIF experiments are found to give fairly repeatable temperature distribution.

3.3.2. High compressed gas pressure

Fig. 6 illustrates another set of experimental results using the simulated flat piston, with an initial pressure of 700 Torr and an initial temperature of
Fig. 5. PLIF intensities and the deduced temperature distributions at varying times after compression for a simulated flat piston head. Gas composition: 2% acetone in nitrogen. Conditions at TDC: pressure = 12.5 bar and temperature = 780 K. Dotted line: raw fluorescence intensity. Dashed line: calculated fluorescence intensity in a uniform temperature field using the Beer–Lambert law. Solid line: deduced temperature distribution.

297 K. The molar concentration of acetone is 1% in nitrogen. This results in the compressed gas pressure of 39.5 bar and compressed temperature of 815 K at TDC. The features of the temperature field are similar to those obtained at the low compressed pressure. Specifically, there exists temperature depression in the center at the end of compression and side depressions appear at the subsequent time steps. In contrast to the measurement at low compressed pressure, at high compressed pressure the central depression in the temperature distribution is smaller, being around 65 K. At the subsequent time steps, the central temperature depression at higher compressed pressure is generally less than that at lower compressed pressure.
3.4. Creviced piston

3.4.1. Low compressed gas pressure

Using a mixture consisting of 1% acetone in nitrogen, a series of experiments with the creviced head piston are conducted. Initial conditions of 275 Torr and 297 K yield compressed gas conditions at TDC of 11.95 bar and 760 K. PLIF results and the deduced temperature distribution at varying time steps are shown in Fig. 7.

At 4.1 ms postcompression, the effect of the vortex has not reached the center of the chamber and the depression in temperature is observed to be approximately 35 K. At 6.2 ms, the central depression corresponds to approximately 30 K, as shown in Fig. 7. However, at 12 ms the effect of the vortex has grown...
In comparison with the case of the flat piston at low pressure, the effect of the vortex is reduced, although it is not eliminated. Fig. 7 also demonstrates that the development of temperature inhomogeneity is relatively gradual for the case of the creviced piston.

3.4.2. High compressed gas pressure

Fig. 8 shows the experimental results for the mixture consisting of 1% acetone in nitrogen, with the initial conditions of 870 Torr and 297 K. At the end of compression, the compressed gas conditions at TDC are 39.5 bar and 770 K. It is seen from Fig. 8 that there is no evidence of any temperature inhomogene-
Fig. 8. PLIF intensities and the deduced temperature distributions at varying times after compression for a creviced piston head. Gas composition: 1% acetone in nitrogen. Conditions at TDC: pressure = 39.5 bar and temperature = 770 K. Dotted line: raw fluorescence intensity. Dashed line: calculated fluorescence intensity in a uniform temperature field by using the Beer–Lambert law. Solid line: deduced temperature distribution.

ity at 2 ms postcompression. The temperature in the chamber is quite uniform and the fluorescence signal shows exponential decay. At the subsequent time steps, even up to 114 ms, there is no effect due to the vortex. Eventually, the effect of the vortex becomes noticeable. At 200 ms, the depression due to the vortex is approximately 40 K, while at 390 ms the central depression corresponds to approximately 100 K.

These results clearly show the effects of the pressure and piston head design on the aerodynamics within an RCM. In comparison to the results using the creviced piston at low pressure (Fig. 7), at high pressure the effect of the vortex roll-up is significantly reduced. While at low pressure the effect of the vortex appears from the end of compression, at high pressure such an effect becomes noticeable only at time
greater than 114 ms postcompression. Furthermore, in comparison to the results using the flat piston at high pressure, the creviced piston at high pressure yields a much higher degree of homogeneity inside the test chamber for long time duration.

4. Numerical analysis

Star-CD CFD package is used to simulate the experimental conditions and provide insights into the detailed evolution of the aerodynamic field inside an RCM. As with the experimental tests, simulation is conducted for conditions of low, intermediate, and high compressed gas pressures, and for the flat as well as the creviced piston head configurations.

Because of the cylindrically symmetric geometry of the combustion chamber, numerical simulation is carried out on an axisymmetric grid distribution. In the actual physical situation in the RCM, flow may deviate from axisymmetric behavior and exhibit asymmetrical patterns. However, axisymmetric configuration is nevertheless chosen because it considerably reduces the computational time while capturing the essentials of the underlying fluid dynamics. Computations are performed from the beginning of the compression stroke with a compression time of 30 ms. Initially, the test gas, nitrogen, at rest is specified with uniform temperature and pressure. A constant temperature of 297 K and no slip condition are specified at the cylinder wall boundary and piston surface.

In the simulation, the piston starts from rest and its motion is given in a manner similar to the piston motion in an engine, by specifying dimensions for the crank radius and the connecting rod length. This specification of velocity profile is consistent with the operation of the present RCM, in which the piston accelerates from rest initially, eventually decelerates at a constant rate, and comes to a stop due to the hydraulic stopping mechanism. Furthermore, by varying the crank radius and the length of the connecting rod in the CFD calculations, it is observed that as long as the compression time is kept constant, the resulting flow field is insensitive to reasonable changes in the velocity profile. This observation is consistent with the finding of Würmel and Simmie [14]. At top dead center, the piston comes to rest and remains there for subsequent time steps. A time step of 55.55 µs is taken, as further reduction of the time step by a factor of two results in identical solution. During the compression stroke, the vertex filling methodology of Star-CD [19] is chosen for the motion of the grid. In this method, the same number of grids is maintained between the cylinder head and the piston head, but the grids become compressed as the piston moves. After the end of the compression stroke, the computational grids remain the same for the post compression period.

The computational grid distribution employed for the creviced piston configuration at the end of compression is shown in Fig. 9. The main reaction chamber consists of 100 grids in the radial direction and 140 grids in the axial direction. In the radial direction, the finer grids are used near the boundary. In the axial direction, an accordion distribution is used, with the finer grids near the piston and cylinder head and the coarser grids in between. In order to ascertain the quality of the grid distribution, selective cases are calculated on a finer grid distribution of $150 \times 200$ in the radial and axial directions, respectively. The use of the finer grids results in an identical flow pattern and less than 0.25% change in predicted temperature. As a result, all the computed results shown herein are obtained on a $100 \times 140$ grid distribution.

In addition, calculations are performed and compared for both laminar and turbulent flow conditions. Since it cannot be easily ascertained a priori whether the postcompression flow field inside an RCM is laminar or turbulent, it is important to perform calculations using both laminar and turbulent models, and assess their predictions by comparing with the experimental results. Various turbulent models are considered. A standard version of the $k-\varepsilon$ model is found to yield extremely high turbulent mixing. On the other hand, calculations using a RNG model yield relatively less turbulent mixing and are found to be closer to the experimental observation in comparison to the results obtained using the $k-\varepsilon$ model. Furthermore, computational results show that the features of aerodynamics are better predicted by laminar calculations, while the actual aerodynamic pattern is expected to be some-
where in between the laminar and turbulent calculations.

5. Computational results

Using the flat piston, Fig. 10 shows the computed fields of velocity and temperature for various time steps after the end of compression under laminar conditions. This is the case with a relatively low compressed pressure of 12.8 bar at TDC. At the end of compression, i.e., at 0 ms, maximum velocity in the chamber is 12.33 m/s. There is a big vortex spanning almost the entire chamber, which shears cold gases from the boundary and brings them inside. As
such, the regime near the centerline is greatly affected by the flow of the cold gases from the boundary. Along with the main vortex, the computed results show the formation of corner vortices near the cylinder wall, the piston head, and the centerline. At 20 ms after compression, the maximum velocity has reduced to 3.27 m/s, but the velocity pattern is markedly different from that at the end of compression. The corner vortex on the piston head also becomes significantly large. At the subsequent time steps, the pattern of the flow field remains almost identical and the velocity in the chamber continues to decay. At 60 ms, the maximum velocity is reduced to 1.19 m/s.

As a comparison, Fig. 11 shows the computed results using the RNG turbulent model under similar conditions of Fig. 10. The compressed pressure at TDC is now 13.14 bar. For this turbulent simulation, the maximum velocities at the end of compression (0 ms) and at 10 ms postcompression are respectively 13.38 and 5.48 m/s, which are not much different from those of the laminar simulation. However, the turbulent calculations do not exhibit any corner vortex, as seen in the laminar model. This is expected as turbulence suppresses the onset of flow separation. Fig. 11 also demonstrates that the nature of velocity field remains identical for all the time steps calculated. In the temperature field, enhanced mixing and
shallow temperature gradient are shown in Fig. 11, as compared to the laminar results.

When comparing PLIF data with the computational results, it can be clearly seen that the simulation using the laminar model agrees well with the features of the aerodynamics observed in experiments, whereas the turbulent calculations fail to do so. The existence of sharp temperature gradients in the experimentally deduced temperature profile is also shown in the laminar flow calculations. It should be mentioned that although the turbulent calculations may not completely capture the qualitative trend observed in the PLIF experiments, the comparison of Figs. 10 and 11 provide insights into the effect of turbulence on the aerodynamics inside an RCM.

As with the experimental results, the effect of the vortex on the temperature distribution near the central portion of the chamber at the end of compression is also noted in the numerical simulation. However, depression in the temperature predicted by the simulation is greater (200 K) than that obtained by the experimental data (100 K). This quantitative difference can be attributed to a number of reasons as follows. The piston used in the experiment is a simulated flat piston with approximately 10% of the crevice volume and not a truly flat piston as employed in the simulation. Therefore, relatively smaller effect of the vortex in the experiment than what would occur for a truly flat piston for which simulation is calculated is expected. In addition, simulation is conducted for conditions of constant wall temperature. But in the actual experiment, it is expected that the wall temperature increases by a few kelvin, resulting in smaller temperature nonuniformity.

Furthermore, there exist alternating hot and cold regions in the experimental results using the flat piston (cf. Figs. 5 and 6). Moving from the wall boundary toward the center, there is a zone of high temperature. After this zone, there is a low temperature regime, followed by another zone of high temperature. Finally, the center of the chamber is at low temperature. Such a temperature field can be produced only by multiple vortices, rotating in different directions. Similar features can be observed in the computed temperature and velocity fields at 20 ms for the laminar calculations, as shown in Fig. 10b. There are alternating hot and cold regions and the velocity field exhibits primarily two vortices.

Based on the laminar calculations, Fig. 12 shows the computed temperature and velocity fields for the creviced piston at a relatively low pressure of 11.9 bar at TDC. For the ease of representation, only the main chamber volume, apart from the crevice zone, is shown in Fig. 12. At the end of compression (0 ms), there is small temperature nonuniformity near the piston head. The maximum predicted gas velocity at this time is 2.29 m/s, which is much smaller than the gas velocity for the flat piston. The effect of the vortex is seen to gradually grow at the subsequent time steps. Even at 80 ms post compression, unlike the flat piston case, significant part of the chamber is unaffected by the vortex, as shown in Fig. 12c.

Fig. 13 shows the simulated temperature fields for the flat piston at a higher pressure of 40.7 bar at TDC, using the laminar model. Patterns of the velocity and temperature fields are identical to those calculated at low pressures. However, at higher pressures, the effect of the vortex penetrates at a much slower rate. For instance, the temperature distribution at 40 ms under a higher compressed pressure (Fig. 13c) is very similar to that at 20 ms under a lower compressed pressure (Fig. 10b).

Compared with Fig. 13, Fig. 14 shows the laminar simulation for the creviced piston at a similar compressed pressure of 39.9 bar at TDC. At the end of compression, apart from minor nonuniformity at the center, the effect of the vortex is practically nonexistent. At the postcompression time of 100 ms, the vortex effect eventually reaches the central plane of the chamber. Similar features are observed in the experimental results. However, the laminar calculations predict an earlier onset time of the temperature inhomogeneity, as the experimental results do not observe any apparent vortex effect until 114 ms post compression.

In addition, the effect of pressure on the vortex formation for the creviced piston is consistent in both the experimental and computational results. Increase in pressure reduces the effect of the vortex. For a flat piston, although such a pressure effect cannot be clearly observed in the experimental data, it is demonstrated in the computational results. The effect of pressure on the vortex roll-up and the induced temperature inhomogeneity can be attributed to the change in the thermal diffusivity. At a higher compressed gas pressure, the mixture thermal diffusivity is lower, thereby leading to a thinner thermal boundary layer. Since temperature inhomogeneity is induced by the shearing of cold gases from the boundary to the interior of the cylindrical chamber, a thinner boundary layer under high compressed gas pressures will slow down the development of the temperature inhomogeneity.

6. Assessment of the adiabatic core hypothesis

The adiabatic core hypothesis is based on the assumption that the effect of heat loss due to the chamber wall does not affect the temperature of the core region at the short time scales encountered in an RCM. From the present experimental results using both flat
For the case of flat piston at a low pressure, at the end of compression (Fig. 5a) there is large temperature gradient at the center of the chamber, while the rest of the chamber is not much affected. However, at the post compression time of 6 ms (Fig. 5b), the temperature gradient is present across the entire chamber. This indicates that the temperature gradients do not completely vanish at the end of compression. With the creviced piston heads, the validity of the adiabatic core hypothesis can be clearly identified.
domain of the chamber and the effect of rolled-up cold gases has spread everywhere. Therefore, at 0 ms there is a possibility that the adiabatic core assumption may hold, but the actual temperature quickly begins to deviate from the adiabatic core temperature. From 6 ms onward, the failure of the adiabatic core hypothesis is expected. For the flat piston at a high compressed pressure, the temperature gradient across the entire chamber is observed at 15.8 ms postcompression (Fig. 6c).

For the case of creviced piston at a high pressure, even at 114 ms post compression (Fig. 8f), the effect of the vortex is not observed. This suggests the validity of the adiabatic core assumption up to this time when using the creviced piston at high pressures. However, at low pressures, the validity of the adiabatic core hypothesis may not be as good.

Similar features regarding the validity of adiabatic core hypothesis are also observed in the computational results. Fig. 15 plots the time evolution of the temperature, the pressure and the maximum temperature, obtained from the simulations employing different conditions and piston head configurations. In addition, the temperature profile calculated by using the adiabatic core hypothesis is also shown and compared. In Fig. 15, the temperature based on the adiabatic core hypothesis is deduced from the corresponding simulated pressure trace. At the end of compression (0 ms), the core temperature predicted by the hypothesis exactly matches with the maximum temperature of the CFD analysis. For the flat piston, however, the computed maximum temperature using the laminar model, shown in Figs. 15a and 15b, quickly begins to significantly deviate from the temperature of the adiabatic core assumption as the postcompression time proceeds. When the turbulent simulation is used, Fig. 15c shows that a larger overprediction resulting from the adiabatic core assumption is observed. In contrast, for the creviced head piston the adiabatic core hypothesis accurately predicts the maximum temperature for a long period of postcompression time, as shown in Figs. 15d, 15e, and 15f.

Fig. 16 compares the extent of the core region from the end of compression simulated using two different piston head configurations, for both laminar and turbulent calculations. Here the core region is defined as the ratio of the volume of the chamber that is within 5% of the maximum instantaneous temper-
Fig. 14. STAR-CD simulation of temperature field at varying times after compression for a creviced piston at a pressure of 39.9 bar at TDC under laminar condition.

ature to the total volume of the chamber at the end of compression. For the case of creviced piston, only the main cylinder volume, apart from the crevice, is considered for the core region calculation. Note that the core region may not be the geometric center of the chamber, but the region of the maximum temperature.

For the flat piston at low pressure of 12.8 bar at TDC, while at the end of compression (time = 0 ms) the core region encompasses approximately 70% of the volume of the chamber, it rapidly reduces to 35% at 20 ms and continues to reduce as the post-compression time proceeds. The present simulation also demonstrates that although relatively large gas volume is at adiabatic core temperature at the end of compression, the heat transport rates from this core region are not low. The failure of the adiabatic core assumption after the end of compression results from the high gas velocity field in a small confined chamber. This can be understood from the time evolution of the maximum gas velocity from the end of compression, as shown in Fig. 17. Significantly higher velocities with the flat head piston in comparison to the creviced piston are seen in Fig. 17. High gas velocities at the end of compression quickly bring the effect of wall into the core region.

For the flat piston at a high pressure of 40.7 bar at TDC, Fig. 16a shows that the extent of the core region is relatively larger than that at a low compressed pressure of 12.8 bar. In contrast, with the creviced piston, the extent of core is significantly increased. Fig. 16b further demonstrates the effect of the turbulence on the extent of the core region. In general, the effect of turbulent mixing lowers the temperature of the core region while increases its spatial extent. It should be noted that under both laminar and turbulent conditions the primary reason for the failure of the adiabatic core hypothesis is due to the mixing of cold gases sheared from the wall boundary with the core region, rather than the heat loss from cold wall itself.

Fig. 17 also illustrates that the use of a creviced piston head substantially reduces gas velocity at the end of compression. As a result, the temperature predicted by the adiabatic core hypothesis matches closely with the actual maximum temperature for long time interval, as shown in Fig. 15. Additionally, the
extent of the core region is greatly improved, as seen in Fig. 16. Since the determination of the core temperature in an RCM is typically indirect, the present numerical experiments therefore demonstrate that it is extremely important to have proper operating conditions and geometric configuration of the test chamber so that the adiabatic core hypothesis is valid.

Although various RCMs have different operating conditions of clearance, stroke, etc., similar features of aerodynamics as observed in this study are expected. Depending upon the extent of the vortex effect, various RCMs would vary in terms of the validity of the adiabatic core hypothesis after the end of compression, although such a hypothesis is expected to be accurate at TDC. This would explain the discrepancies in the reported experimental data from different RCMs, even under similar compressed conditions.

### 7. Effect of the piston head configuration on ignition delay

It has been shown in Fig. 2 that under similar conditions the use of different piston head configurations can lead to different ignition delay. In order to address the reasons, additional simulations and experiments are carried out based on the same compressed gas temperature and pressure for a flat and a creviced piston head configurations. To achieve the same condition at the end of compression, the clearance is increased to account for the absence of the crevice volume in the flat piston case.

Fig. 18 shows the numerical comparison using nitrogen. Although pressure and temperature at TDC are the same for both piston head configurations, the rate of pressure drop for the creviced piston is higher than that for the flat piston. This result is attributed to
results shown in Figs. 15–17, for the flat piston case the adiabatic core assumption is not valid, and the significant effect of the roll-up vortex decreases the core temperature, despite of higher postcompression pressure. The resulting lower core temperature than that determined based on the adiabatic core hypothesis and the higher postcompression pressure for the use of the flat piston will in turn affect the autoignition delay.

Fig. 19 compares the experimental pressure traces using stoichiometric iso-octane/O$_2$/inert gas mixtures for both piston head configurations under similar composition, compressed gas temperature, and TDC pressure. Results for three different adiabatic core temperatures, namely 684, 745, and 878 K at TDC, are compared in Fig. 19. Both the single-stage (878 K) and the two-stage (684 and 745 K) ignition phenomena are clearly shown. Although the compressed pressures at TDC match quite well for both pistons, it is seen in Fig. 19 that the postcompression pressure for
the flat piston is higher, as demonstrated by the computational results. The combined effect of the lower core temperature than that calculated using the adiabatic core hypothesis and the higher postcompression pressure for the flat piston case alters the ignition delay as depicted in Fig. 19.

8. Conclusions

The purpose of this work is to investigate the effects of aerodynamics on the measured properties within a rapid compression machine. Such an understanding is important in order to unambiguously characterize the state of the reacting mixture and to explain the reasons for the mismatch of ignition delay data obtained from various RCMs. Experimental and computational studies are conducted for a flat and a creviced piston head configurations. Experimental results using PLIF of acetone demonstrate the suitability of a creviced piston to provide a homogeneous reacting core. Computational results under laminar conditions closely reproduce the features of the aerodynamics that are observed in the experiment. For a flat piston, although the adiabatic core assumption accurately predicts the temperature at the end of compression, it significantly overpredicts the postcompression temperature as the effect of fast-moving cold gases quickly spreads all over the chamber. A creviced piston head is found to significantly increase the extent of the core region. Therefore, when using a properly designed creviced piston, the postcompression temperature can be accurately predicted based on the adiabatic core hypothesis. It is also observed that the effect of the roll-up vortex is reduced as the compressed pressure is increased.

The present results demonstrate that using a creviced piston design, the actual temperature in an RCM can be deduced from the pressure trace. From the kinetic modeling point of view, unambiguous determination of the temperature is the prime requirement, as the heat loss associated with an RCM can be easily accounted for by using an empirical relation. This work suggests that when a properly designed creviced piston is used, a zero-dimensional model should satisfactorily model the experimental results using an RCM. However, when a flat piston is employed, the use of a zero-dimensional model to simulate the experimental data is deemed inadequate.

Acknowledgment

This work was supported by the National Science Foundation under Grant No. 0133161.

References