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A Single Stroke Cylinder Rapid Compression Machine for Chemical Kinetic Study at Elevated Pressure and Temperatures.

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Abstract

The fabrication of a rapid compression machine (RCM) is in its early phase of design. The machine is designed to enhance the study of ignition delay and validation of detailed kinetics models of fuels. The machine compresses fuel/air mixtures isentropically within 25 to 52 ms with a varying stroke. The combustion chamber design is not fixed and can be adjusted through the threaded shaft lock and within chamber slots. The originality of the facility is the inclusion of a pneumatic piston release mechanism (PPRM), which is pneumatically operated. The current test facility has been characterised by conducting a nonreactive and reactive experiment, the result showed that an obtainable compressed pressure of 21 bar and end gas temperature of approximately 1000 K was achievable within the present facility. The fidelity of the facility was performed with a non-reactive experiment, which experimental pressure profile was seen to follow each other closely showing that the data are highly repeatable within the test condition, the result was free from any form of rebound or disturbance, which would have adversely distort the result. The experiment data was simulated implementing the effective volume approach and was seen to perfectly match with the experiment at both stages of compression. The reactive experiment was demonstrated with heptane/air mixture at stoichiometric condition, $T_C = 625 \leq 689$ K. The results show that the experimental pressure traces overlay each other thus signifying a repeatable pressure trace and this demonstrates that the Shef-RCM is operable and ready at its first stage of design for studying the ignition delay time of liquid fuels operating within an engine like conditions and for validating chemical kinetics models.

Keywords: Ignition delay time; Shef-RCM; Piston Design; Chemical kinetics.

1.   Introduction

In the early 1900s, the first vertical single piston RCM was designed with a without a braking mechanism [1]. The facility was propelled by the transfer of energy from the flywheel drive crank and falling weight [2]. The device lacks a cushioning device that would stop the piston, invariably not maintaining a consistent volume at the Top Dead Centre (TDC). Modern designs of RCM's have multiple features such as; optimised piston crevice [3, 4], hydraulic damper [4], an optically asscessibility [5], species measurement of fuels [2, 6], minimal vibration, cam operated piston [6, 7], pneumatic piston release mechanism [8], external mixing vessel and non-external mixing vessels [7, 9]. Piston speed and control are vital in RCM design. However, the piston speed needs to be fast enough to prevent excessive heat loss from the test facility, so it is pneumatically driven [1, 10]. Since they are pneumatically driven, the reactor piston possesses a high velocity, which needs to be stopped instantaneously and locked in a position at TDC. In

the early designs, various concept was used in stopping the reactor piston these ranges from plastic deformation of metal, air cushion system, using powerful springs and transferring piston momentum to an auxiliary floating mass to absorb piston energy. These methods used are very challenging and difficult to manipulate, therefore offer unreliable results. The more effective means of stopping the reactor piston at TDC is using hydraulic stopping mechanism, which was first proposed by Rogowski [11] and has proved to be more superior to the early designs. Though, the reactor piston is decelerated by letting out hydraulic fluid under pressure through the step surface as the ring as it journeys into the hydraulic groove. Other RCMs design uses an alternative concept of stopping the reactor piston, these include the interference fit of a polymeric piston in the bore of the chamber as reported by Donovan et al. [12] and using the shape of a cam to stop the piston [13]. All the concept displayed ensures that the design maintains a constant volume reaction chamber, where rebound and overshoot should be avoided or minimized.

Compression time plays an important role in the induction time of fuels. Shorter compression time helps to minimize the induction time and prevent reactivity occurring before the end of TDC. Instead of a single piston configuration, most RCMs adopt the dual opposed-piston configuration as early studied by Affleck and Thomas [2]. Their design has the advantage of simultaneously triggering the twin piston to reduce compression time and also maintain mechanical balance.

In RCM experiment, the fuel /air mixtures are compressed relatively close to adiabatic compression but the result deviates from the ideal situation due to loss of heat to the chamber walls. The combustion chambers design comes in various shapes. However, quite a number may be fixed [9, 14], while others are adjustable chamber [7]. The combustion chamber houses some sensing devices such as dynamic pressure transducer, static pressure transducer, thermocouples, the port for charging fuel-air mixtures into the chamber and some designs may have an opaque window for species visualization in the chamber.

Fuel/air mixtures are usually made in a mixing tank before the experiment is conducted [2, 11, 14-16]. This mixing tank should be properly insulated to avoid condensation and thermal stratification of the mixture composition. The technique is more advantageous in that the mixture composition remains unchanged throughout the test condition due to large volumes of the mixtures prepared in the mixing tank in advance of the experiment. In the absence of an external mixing tank, the combustion chamber may be designed to accommodate the fuel/air mixture directly injected into the chamber rather than mixing externally. This type of design is known as the direct test chamber (DTC) [7, 9]. The technique eliminates the issue of condensation of the vapour gas in the pipelines, which may result from poor insulation of the piping network.

The chamber temperature is maintained at the test condition with heat tapes, 6-band heaters [9], wrapped around it and insulated to minimize chamber wall heat losses to the atmosphere. One defect in RCMs design is the formation of the roll-up vortex, which results from the motion of flat piston scrapping cold gases from the chamber walls and then deposit at the centre of the combustion chamber. This phenomenon has led to the mixing of the cold gas from the chamber walls into the vicinity where combustion takes place [17-20]. The vicinity where combustion occurs is referred to the core region. This effect has been studied [14] and computationally investigated [21-24]. However, in a previous study, the piston head with crevice design plays a major role in controlling the phenomenon and sustain the uniformity of the core region in the chamber. The non-uniformity in the core region of the chamber could result in the dissimilar

interpretation of data from different machines and also inefficient heat loss characterization for the related RCMs. Lee and Hochgreb [24] performed a computational study on the aerodynamics in the RCM. In a bit to study the induction time preceding combustion, the multi-dimensional effect should be effectively controlled in order to obtain reliable data for chemical validation.

The chemistry within the region of low to intermediate temperature has relevance in achieving combustion in HCCI engines whereas, in spark ignition (SI), it produces undesirable 'knock' in engines. Comprehensive knowledge and the understanding of combustion chemistry in these regimes are necessary for adequately control of autoignition phenomenon and this has continued to be an interest to combustor designer in achieving a promising engine with low NOx. At that juncture, this work is presenting the first stage of design and fabrication of Shef-RCM, and characterizing it fit for autoignition study and the validation of chemical kinetic models.

2.   Design of the Facility and its Operations

Figure 1, shows a typical diagram of the current Shef-RCM. The pneumatic, hydraulic, and the reactor piston are all connected by an interlinking rod from the pneumatic driver section, which moves as a unit. A Norgren actuator with model number PRA/182/100/M/600 act as the driver section/pneumatic chamber is linked to the high-pressure side of the air compressor. It operates at a pressure less than 11 bar and has a stroke length of 600 mm. The pneumatic chamber is the driver section of the machine, air from the compressor is supply to the pneumatic cylinder, which is used to propel the reactor piston. As a result of the high velocity of the reactor piston, hydraulic damping unit was designed and optimized to effectively slow down the reactor piston until is finally lock in a position at a constant volume. The hydraulic damping mechanism is made of a stainless steel ring and a groove fixed in a hydraulic oil-filled cylinder. The ring was machined in three steps and four holes of 5 mm bore drilled on the exterior surface of the ring. The holes on the surface help minimize the frictional drag and enhance the velocity of the piston. The reactor piston was slowed down was by venting of the high-pressure oil trapped in the groove as the ring travels into the groove, thereby discharging this trapped hydraulic fluid through the step surface of the ring and the drilled holes.

Burning takes in the combustion chamber while the piston is exposed to extreme temperature and pressure. The reactor piston should be designed to have sufficient strength, stiffness, be light weighted and thermally stable with low thermal conductivity. The reactor piston was made of Aluminum alloy 6082-T6, which has a diameter of 39.6mm and 50mm long. When design a piston, the expansion coefficient should be low as possible to avoid the piston freezing in the chamber when exposing to extreme temperature. However, the present piston expansion was within the clearance of 0.2 mm. The piston head design configuration plays a major role in sustaining a homogeneous temperature profile and minimizing the non-ideal influences such as roll-up vortex and non-uniform heat release in RCM. Based on Mittal design [25] the piston for the present machine was optimized using CFD package as reported from the previous work [8, 26]. The distance travelled by the reactor piston was measured with the Linear Variable Displacement Transducer (LVDT), (model DCTH 4000C). The LVDT is a transducer, which changes the linear piston motion to a conforming electrical signal in volts. The LVDT was connected to the reference plate of the machine mounted on the base of the rig frame.

The combustion chamber was designed to accommodate a maximum pressure of 100 bars. It is consist of a cylindrical tube connected to stainless steel blocks. The cylindrical steel tube fits into the block to form the chamber's assembly. A carbonized copper gasket was placed between

the cylinder and the block to maintain an airtight condition inside the chamber. The combustion chamber was designed to accommodate two inlet ports, one for admitting fuel-air mixtures while the other port allows the inflow of air into the combustion chamber at high-pressure, which is used to retrieve the piston after each runs. The innovation of the Shef-RCM design is the PPRM, which controls the machine. It acts as the break, holds and releases the reactor piston in its initial start position. The operating pressure of the PPRM is within 3-5 bars. It is driven pneumatically and control by a solenoid valve, which engages and disengages the shaft piston lock. The combustion chamber temperature is maintained with a heating tape (Omegalux) bound around the chamber and regulated by a PID controller coupled to the K-type thermocouple positioned at the back of the combustion chamber.
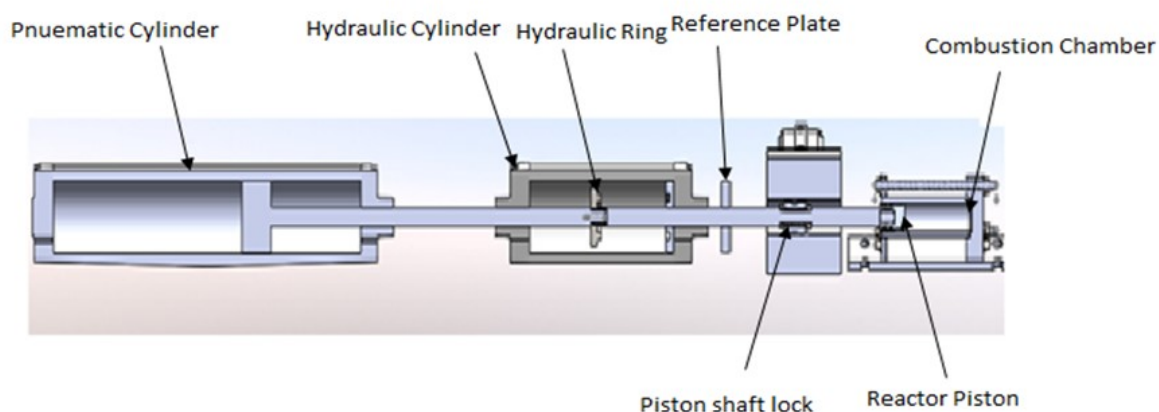

Figure 1: Shows the University of Sheffield RCM (Shef-RCM) test facility

2.1 Experimental Procedure

A BOC Edward E2-M12 vacuum pump was initiating used to vacuum the combustion chamber and intermittently injected with 50 ml nitrogen to get rid of the air in the combustion chamber. The composition of the fuel / air mixture was prepared based on the molar composition before charging the combustion chamber. Gases mixtures (pure oxygen and nitrogen) of purity 99.9% was kept in a Teflon FEP gas sampling bags of about 600 ml. The required composition was extracted using a 50 ml syringe for the gas and a 50 ml micro-syringe for liquid fuel. At the specific condition, the fuel/air mixtures was charged into the heated combustion chamber from the inlet port position at the back of the chamber via a septum and the mixtures left to homogenize for about an hour and half. For this experiment, five bar driver pressure was used behind the driver unit to drive the reactor piston, which was activated by disengaging the PPRM, then compresses the fuel/air mixtures to elevated pressure and temperature. The events were logs onto the LabVIEW and later retrieve for further processing. The piston was retracted to its initial position, BDC then the combustion chamber cleaned after every three runs with propanol and subsequent pressurising of the chamber with air up to 1.5 bar from the compressor and finally vacuum for about 5-7 minutes, then the rig is ready for the next runs of the experiment. The compressed pressure at TDC was varied by altering the compression ratio or the initial pressure of the mixture, while the end gas temperature was altered by one of the following ways adjusting the initial temperature, compression ratio and mixture specific heat. The only variable measured from the experiment was the pressure traces, recorded by the dynamic pressure signal using a piezoelectric sensor (Kistler 6009 and a charge amplifier (Kistler type 5007). The data

acquisition was recorded with NI cDAQ 9223. The temperature sensor and the heating tape are connected to the PID controller, where the initial temperature readings are recorded.

2.2 Autoignition Definition

The expected results of an RCM test are the ignition delay times, which must be properly defined in order not to be misleading. The ignition behaviours are reflected in the reactive experimental results illustrated in Figure 2; this shows typical pressure history for *n*-heptane/air mixtures at the ɸ= 1. The definition of ignition delay appears to have one peak pressure rises signifying a single stage ignition of n-heptane oxidation. The zero time corresponds to TDC at 17 bars. *P(t),* is define as the experimental pressure profile as a function of time where P'(t), is the first derivative of the pressure profile as a function of time. τ_1 is gives the first stage of ignition delay from the time at TDC to the peak in the time derivative of the pressure [27].
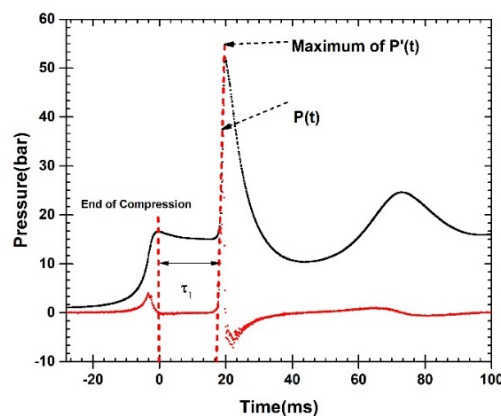

Figure 2: Shows the description of ignition delay used in this study. P(t) is the pressure as a function of time, and P′(t) is the time derivative of the pressure as a function of time.

3.   Result and discussions

3.1   Facility Characterization

four different runs were conducted for non-reactive tests was by expanding inert gas (nitrogen and argon) and a reactive test using heptane/air mixture in the heated combustion chamber. Data acquired was experimental pressure profiles which were recorded on LabVIEW and represented as pressure profile versus time history as display in Figure 3.

Figure 3(a) depicts the pressure trace for a non-reactive test (nitrogen and argon) at P_C = 18.2 and 21 bar. Figure 3(b) shows the pressure traces of a reactive test for heptane/air mixtures at ɸ = 1. The raw pressure data taken from the facility are not affected by any disturbances or vibrations. The pressure profile for both reactive and non-reactive test were seen to overlap and follow each other thus demonstrating a repeatable an experimental pressure traces. The absence of a rebound in the pressure data has demonstrated the effectiveness of the hydraulic stopping mechanism.
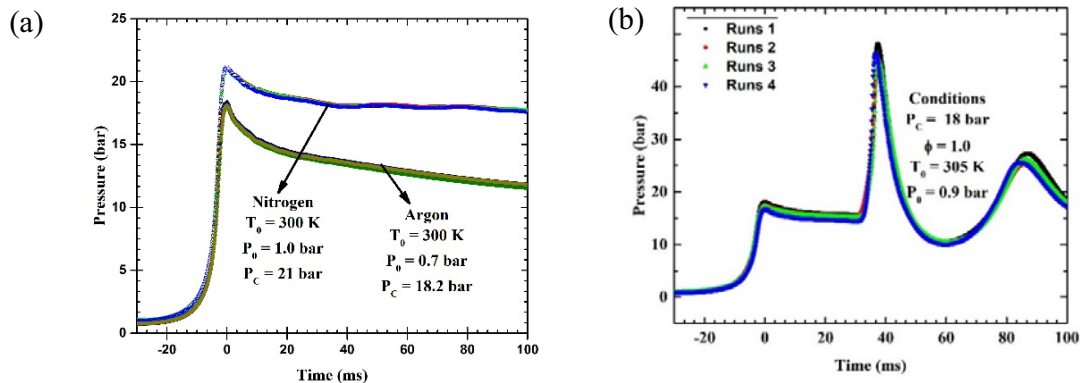
Figure 3: display the experimental repeatability test (a) Non-reactive test using nitrogen and argon gas.(b)Experimental repeatability of n-heptane/air mixture, molar composition: $nC_7H_{16}/O_2/N_2 =1/11/41.36$.

Figure 4 depicts the plot of experimental pressure profile as a function of time for Heptane/air mixtures at a peak pressure of 20 bar and end of gas temperature $625 \leq \phi \geq 689$ K, for $\phi = 1.0$. The time 0 corresponds to TDC. The non-reactive experiment was carried out for the same condition and mixture composition by replacing the O_2 with N_2. The pressure profile clearly showed that the pressure trace after post-compression is not constant but decayed gradually as a result of the heat loss from the fluid to the combustion chamber wall. The influence of compressed gas temperature is seen on the induction time. The ignition delay time is seen to decrease as the end of compressed gas temperature (EOC) is increased.
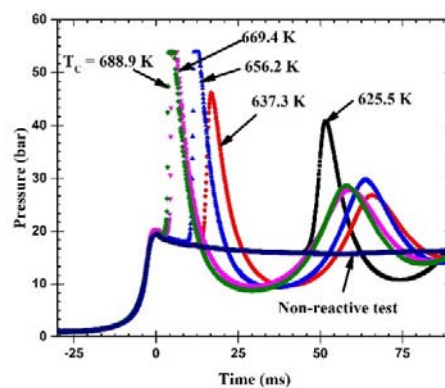

Figure 4: Shows the effects of EOC temperature on the Ignition delay time for Heptane/air Condition; $\phi = 1.0$ at $P_c = 20$ bar and oxidizer to mass ratio of 14.6.

Figure 5, depicts the measured ignition delay for Heptane/air mixtures at stoichiometric condition as a function of compressed temperature. The plot shows that increase in the compressed gas temperature leads to the corresponding reduction in the ignition delay. This clearly displayed an Arrhenius-like temperature dependence with no NTC behaviour.
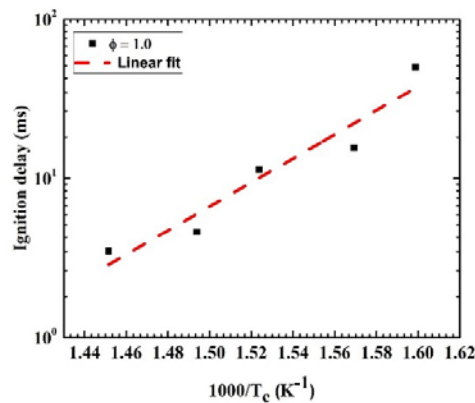
Figure 5: (a) Shows the measured ignition delay as a function of compressed gas temperature. Condition; ф = 1.0 at P_c = 20 bar and oxidizer to mass ratio of 14.6.

3.2 **Temperature Estimation and Numerical Modelling**

The peak temperature T_c at TDC cannot be estimated directly, because of the slow thermal responses of the thermocouple due to the rapid heat loss from the fluid to the walls of the combustion chamber. Rather, an adiabatic core hypothesis is assumed as described in the literature [28, 29] was used to calculated the T_C from experimental pressure trace. This theory performs well, if the multi-dimensional influence such as rolls up vortex and heat loss are handle using an optimized piston crevice design. The theory assumes that the influence heat loss to the wall during compression is restricted to thin boundary layer along the wall of the combustion chamber and the region away from the wall is not affected by heat loss. The region of the chamber not affected is referred to the core region. Nevertheless, this region is assumed to be characterized with temperature uniformity. This assumption of the adiabatic core hypothesis accurately estimated T_C , from the experimental pressure trace according to the relation

$$\int_{T_0}^{T_c} \frac{\gamma}{\gamma-1} \; \frac{dT}{T} = ln\left(\frac{P_C}{P_0}\right) \qquad (1)$$

Where T_0 and P_0 are the initial temperature and pressure respectively, P_c is the end of compressed pressure, γ is the specific ratio.

The more convenient way to model the RCM close to reality is the use of zero-dimensional (O-D) model proposed by Mittal et al. [30], which accounts for the effect of heat loss at both stages of compression. With the use of a creviced piston, the uniformity of the core region is guaranteed and the fidelity of (O-D) model is further enhanced. Other techniques for modelling heat loss in RCM includes incorporating heat loss term in the energy equation while maintaining the constant volume [31] and implementing the multi-zones model proposed by Goldsborough et al.[32]. Nevertheless, in this study, the (O-D) code was adopted to model the RCM such as Cantera[33] in conjunction with the adiabatic volume expansion [25, 28].

The heat loss parameter was derived from the non-reactive experimental pressure history through the effective volume approach as described in the literature [25, 34] by conducting a non-reactive experiment under similar conditions as the reactive experiment replacing O_2 with N_2 and implementing the corresponding heat loss parameters derived for the compression and

post-compression stroke. To match the simulated pressure with the experiment up to the point at TDC during compression, an empirical parameter is included in the time-dependent geometric volume of the combustion chamber. This empirical parameter, therefore, simulates heat loss during the compression period. After TDC, according to the adiabatic core assumption, the volume expansion is specified in terms of a polynomial fit to define the effective volume after compression. Therefore the effective volume history can be calculated as

$$V_t = V_0 \left(\frac{P(0)}{P(t)}\right)^{1/\gamma} \qquad (2)$$

Where $V_{(0)}$ is the volume at the end of compression, $P_{(0)}$ is the pressure at TDC, $P_{(t)}$ is the experimental pressure as a function of time and γ is the mixture specific heat as a function of temperature.

Using the mixture specific heat ratio (as a function of temperature) and the adiabatic core relationships, the measured experimental pressure history from the non-reactive experiment is directly converted into a volume history.

Figure 6, depicts a comparison experiment pressure trace and model for a non-reactive. It shows the pressure history for Nitrogen and Argon used as a test gas. The results show that T_c is less than T_{ac} (adiabatic), in practice, the system is not truly adiabatic, heat is loss from the fluid to the walls of the chamber, which is seen by the gradual decay of the pressure trace at post compression. The model is in good agreement with experiment at both stages of compression.
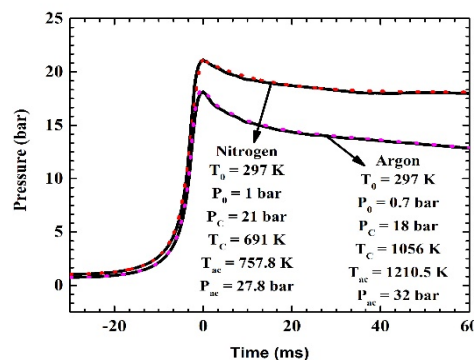

Figure 6: Model comparison with experimental data of a non-reactive test for Nitrogen and Argon gas: model – broken lines, Experiment – Black lines.

Figure 7, depicts the pressure trace as a function of time for a reactive mixture of heptane/air at the stoichiometric condition in a heated combustion chamber compared with different models found in the literature. The experimental data are represented in broken and black lines, while the coloured solid lines represent kinetic models. Two chemical kinetic models, a detailed and reduced mechanism developed by Mehl et al.[35] and skeletal mechanism designed by Luong et al.[36] was used for the simulation. It can be seen that the pre and post-compression heat loss was adequately model, which have good agreement with experiment. The model and experiment displayed a single stage ignition delay, however, the models anticipated a longer ignition delay time compare to the experiment, and this discrepancy is ascribed to the dearth of the reaction mechanism below the conditions of a relatively low compressed temperature of 640 K.
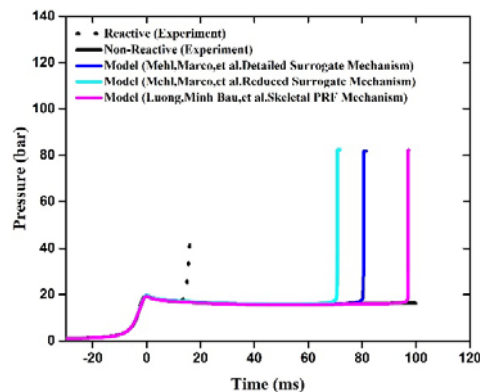
Figure 5: Comparison of different models in literature with experiment data. Condition: n-Heptane/air mixtures at stoichiometric, P_C = 20 bar and T_0 = 315 K. Experiment – Black broken line, Non-reactive – Blackline, Models – Coloured lines.

4.   Conclusion

An RCM has been developed, which has similar features in literature. It is pneumatically operated, hydraulically stopped and compresses fuel/air mixture to a high temperature and pressure of about 20 bar and 1000 K nearly adiabatic. The pneumatic cylinder, hydraulic unit, the reactor piston and the combustion chamber piston are connected to a single shaft. The piston profile of the facility was measured with the linear variable displacement transducer(LVDT) synchronised to the RCM. The combustion chamber is not fixed but could be adjusted within its slot to vary the compression ratio. The speed of the reactor piston was gradually slow down with the assistance of the hydraulic ring and groove mechanism unit until it gets to the end of TDC, which maintained a constant volume at end of the stroke. The facility was designed with a replaceable piston head, which gives rooms for a variety of optimized piston head. The facility was characterized experimentally carrying out a non-reactive test with Nitrogen and argon gas while the reactive test was conducted with heptane/air mixture at ϕ = 1. The repeatability of both experimental tests shows the effectiveness of the hydraulic damping mechanism and the reliability of the experimental data.

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