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Effect of crevice mass transfer in a rapid compression machine

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A B S T R A C T

Rapid Compression Machines (RCMs) often employ creviced pistons to suppress the formation of the roll-up vortex. However, the use of a creviced piston promotes mass transfer into the crevice when heat release takes place in the main combustion chamber. This multi-dimensional effect is not accounted for in the prevalent volumetric expansion approach for modeling RCMs. The method of crevice containment avoids post-compression mass transfer into the crevice. In order to assess the effect of the crevice mass transfer on ignition in a RCM, experiments are conducted for autoignition of isooctane in a RCM with creviced piston in the temperature range of 680–940 K and at compressed pressures of ∼15.5 and 20.5 bar in two ways. In one situation, post-compression mass transfer to the crevice is avoided by crevice containment and in other it is allowed. Experiments show that the crevice mass transfer can lead to significantly longer ignition delays. Experimental data from both scenarios is modeled using adiabatic volumetric expansion approach and an available kinetic mechanism. The simulated results show less pronounced effect of crevice mass transfer on ignition delay and highlight the deficiency of the volumetric expansion method owing to its inability to describe coupled physico-chemical processes in the presence of heat release. Results indicate that it is important to include crevice mass transfer in the physical model for improved modeling of experimental data from RCMs without crevice containment for consistent interpretation of chemical kinetics. The use of crevice containment, however, avoids the issue of mass transfer altogether and offers an alternative and sound approach.

1. Introduction

In response to the increasing global demand for energy and emphasis on efficiency and emission characteristics of practical engines, there is increased focus on developing innovative, efficient, sustainable and clean-burning approaches. Various advanced combustion strategies [e.g. 1–5] share the common denominator of dilute, high pressure, low temperature combustion. This combustion regime is different from the traditional SI and CI engines and operation at these low temperature strategies is significantly kinetically-influenced by the complex low temperature chemistry of hydrocarbon fuels. Therefore, an important ingredient for the design of efficient engines is the need for understanding the chemical kinetic mechanisms of fuels at low temperatures and high pressure conditions. Common facilities for studying homogeneous gas phase chemical kinetics at low temperatures include shock tubes, combustion bombs, flow reactors, jet-stirred reactors, motored engines, and Rapid Compression Machines (RCMs). Flow reactors and jet-stirred reactors are typically used with highly diluted mixtures, whereas RCMs and shock tubes allow observation of autoignition at appropriate fuel loading.

Autoignition at low temperatures can be influenced by phenomena that are facility specific [6]. In shock tubes for instance, experiments at low temperatures can manifest pressure rise due to shock attenuation. In addition, significant fuel-specific pre-ignition behavior is sometimes noted where ignition is non-homogeneous initially, and is followed by a pronounced deflagrative phase, compression of the unburned mixture and the eventual autoignition. The induction chemistry can be highly sensitive to the perturbation from shock attenuation and deflagrative phase and the consequent pressure increase can shorten autoignition delay even by an order of magnitude [7]. Therefore, ignition delays reported without any pressure histories can be highly misleading and could lead to misinterpretation of the experimental data at low temperatures. On the other hand, observed ignition delays in RCMs at low temperatures are typically longer than in shock tubes owing to the conspicuous absence of pressure rise due to shock attenuation that is manifested in shock tubes [6,7]. Therefore, the objective is not to ensure that the experimental data from all facilities should match, but to adequately model the facility-dependent and coupled physico-chemical processes to achieve consistent interpretation of experimental data across various facilities for validation of chemical kinetic mechanisms.

In regard to shock tubes, the effects pertaining to the shock attenuation and deflagrative phase have been satisfactorily

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modeled for interpretation of chemical kinetics [6]. For RCMs, experimental data even under similar conditions of compressed gas temperature and pressure from various RCMs differs due to the facility dependent fluid dynamics and heat loss characteristics [8]. Apart from the surface area to volume ratio of the combustion chamber which directly governs heat loss, RCMs can be classified into three categories based on the configuration of the end combustion chamber – flat piston, creviced piston and creviced piston where crevice is also contained at the end of compression. The corresponding physical processes are also different. Use of a flat piston leads to enormous piston motion induced roll-up vortex and temperature non-homogeneity [9–17]. This fluid mechanical effect is particularly complicated because it does not even show up in the pressure trace and there is no easy way to account for it. With a creviced piston, the roll-up vortex is avoided; however, mass transfer to the crevice during heat release in the main combustion chamber can become problematic [17–21]. Crevice containment allows suppression of the vortex during the compression stroke while avoiding the issue of mass transfer to the crevice during the post-compression period [18–20].

Regardless of the type of RCM, the modeling to account for the compression stroke and post compression heat loss is mostly conducted by using an adiabatic core hypothesis [17,22–24]. This hypothesis assumes no mixing between the cold boundary layer and the hot core region, and the only way the effect of near-wall heat loss penetrates the core region is through the expansion of the core region caused by the cooling of the boundary layer. Therefore, even though the geometric volume of reaction chamber remains unchanged after the piston reaches the end of compression, the core region experiences an expansion that can be modeled as adiabatic volume expansion and the ‘effective volume’ of the core region can be derived from the non-reactive pressure trace. For every reactive experiment, this method requires an experiment with a non-reactive mixture of the same heat capacity and thermal conductivity as the reactive mixture to deduce volumetric expansion parameters. This empirical approach has been very successful for conditions where heat release before hot ignition is not substantial, whereas discrepancy, owing to the non-uniform heat release in the core, boundary layer and crevice, is anticipated when substantial heat release occurs before hot-ignition [18,21,25–27].

In addition, computationally efficient physics based multi-zone models, which enable simulation with detailed chemistry while accounting for the non-uniform temperature due to the cold boundary layer and crevice zone, have also been described recently [21,27]. In comparison to the volumetric expansion approach, which can precisely describe the non-reactive experiment for any RCM, such models might fail to accurately describe non-reactive pressure trace across a range of RCMs with variation in surface area/volume ratio, stroke length, crevice geometry and compression time, even though they can successfully capture the coupling between the chemical and physical processes. A precise description of the non-reactive pressure trace is an advantage of the volumetric expansion approach and the required non-reactive experiments are fast and easy to conduct as well as allow purging of the RCM after each reactive experiment. A hybrid model capable of precisely describing the non-reactive experimental pressure trace as well as the coupling between physical and chemical processes will be most desirable. Such a model is yet to be proposed and at this time the volumetric expansion approach remains the most widely used.

In regard to RCM experiments and modeling via volumetric expansion approach, this work aims to address the following. (i) What is the influence of the crevice mass transfer on experiments in an RCM? Some computational studies have implied an increase in the ignition delay owing to the crevice mass transfer [18,27]. An experimental study of the same is desirable. (ii) Can experimental data in an RCM with a creviced piston be satisfactorily modeled by using the prevalent volumetric expansion approach under conditions of significant heat release before hot-ignition? The answer to this question is very important to validate/ invalidate the prevalent modeling approach. It will be presented in due course that the effect of crevice mass transfer can be enormous, rendering the volumetric expansion approach inadequate.

The above issues are addressed by studying autoignition of isooctane in an RCM by using a creviced piston with and without crevice containment. Isooctane is selected because its low temperature kinetics is most mature amongst all the components that are considered in surrogate formulations, and a comparison of the experimental data and modeling using kinetic mechanism can help answer the above mentioned questions. In the following, the experimental facility is first described followed by the experimental results and comparison with model predictions.

2. Experimental specifications

Experiments were conducted in an RCM. The conceptual design of the present RCM is based on several other RCMs reported in the literature that utilize hydraulic motion control and damping, such as [28–30]. Except for some unique and notable differences, the detailed design of the present RCM is based on the one designed and used extensively by Mittal and Sung [31]. As shown in Fig. 1, the experimental facility is divided into three main components: the pneumatic driving system, the hydraulic system, and the compression and combustion chamber. The pneumatic system consists of a driver cylinder with a bore of 15.24 cm connected to a 75.6 l air tank. The driver cylinder performs two distinct functions. First, it drives the entire piston assembly and prevents its rebound after the end of the compression stroke. Second, it helps retract the piston assembly to its initial position after every run. The hydraulic system consists of a hydraulic chamber, hydraulic piston, pump and lines for filling, draining, and a solenoid release mechanism for firing the machine. The stopping of the piston at the end of the compression stroke is achieved by hydraulic damping.

A stepped reaction chamber geometry is used wherein the combustion chamber (bore 4.67 cm) is connected to the compression cylinder (bore 5.08 cm) through a gradually converging section. A stepped geometry, as incorporated in other RCMs [32–34], can potentially exacerbate vortex formation. The configuration of the present RCM, however, was optimized by CFD analysis [19] to reduce this effect as much as possible. This design also allows for crevice containment. The compression stroke can be varied between 20.32 and 30.48 cm and the clearance volume is also adjustable allowing a range of compression ratios up to 16. The combustion chamber is equipped with the sensing devices for measuring pressure and temperature, and gas inlet/outlet ports for filling gas. The dynamic pressure during the experiment is measured using a piezoelectric sensor (Kistler 6052C) and a charge amplifier (Kistler 5010B). Further, the pneumatic-hydraulic driving system is designed to allow compressed pressures up to 100 bar and combustion chamber is designed to withstand post-combustion pressures up to 500 bar. The test mixture is first prepared manometrically inside a 19 l stainless steel tank that is equipped with a magnetic stirrer and is allowed to homogenize before feeding to the combustion chamber.

As shown in Fig. 1, the compression piston incorporates a crevice and a seal on the piston taper surface to enable ‘crevice containment’. This seal engages with the taper surface on the combustion chamber only near the end of the compression stroke and separates the main combustion chamber from the crevice during the post compression duration. The details of the CFD analysis to arrive at the optimized combustion chamber configuration were presented in [19,20]. The optimized geometry consists of a crevice