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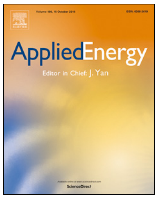

A multizone model of the combustion chamber dynamics in a controlled trajectory rapid compression and expansion machine (CT-RCEM)

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HIGHLIGHTS

- A multi-zone model for the controlled trajectory rapid compression and expansion machine.
- A systematic approach for evaluating the impact of the thermodynamic path on combustion characteristics.
- A framework for evaluating chemical kinetics for various fuels.

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ABSTRACT

A novel, controlled trajectory rapid compression and expansion machine (CT-RCEM) with the unique capability of precise motion control of the piston has been developed. The compression and expansion profile can be varied, in the CT-RCEM, by digitally changing the piston reference trajectory assigned to the active motion controller. Besides the ease of operation, and wider selection of operating parameters with higher resolution, this capability lowers the turnaround time between experiments by eliminating the need for any hardware intervention. More importantly, this capability allows us to tailor the thermodynamic path of compression (and expansion) – essentially the pressure and temperature profile – by appropriate selection of the piston trajectory. However, to effectively leverage these features of the CT-RCEM, a numerical model is essential – for selection of appropriate thermodynamic path for chemical-kinetic investigations, as well as for the interpretation of the corresponding experimental results.

In this work, we present a computationally efficient, physics based multi-zone model of the combustion dynamics of the CT-RCEM, which accounts for the heat loss and piston crevice flows. We show that the concurrent use of the proposed model with the CT-RCEM allows, for the first time, a systematic investigation of the effect of changing piston trajectory – and consequently – the thermodynamic path of compression on the auto-ignition characteristics of fuels. The effect of changing piston trajectory on autoignition characteristics of di-methyl-ether (DME) observed in CT-RCEM experiments has been explained using the proposed model. The study clearly shows that changing the piston trajectory can significantly affect the measured ignition delay due to the resulting change in the thermodynamic path. Also, a shorter compression time for a given compression ratio does not necessarily guarantee smaller reaction progress during compression. The paper concludes by summarizing the unique insight obtained from this study —the use of CT-RCEM for auto-ignition investigation involving thermodynamic paths with similar pressure and temperature conditions at the end of compression but different intermediate species buildup can potentially provide additional information vital for further understanding of the chemical kinetics.

1. Introduction

The ever-increasing energy demands and growing environmental concerns worldwide have given a significant push to the research effort for better understanding of combustion processes in internal combustion (IC) engines. In the U.S alone, the transportation sector, which is dominated by IC engines, accounts for about 28% of total energy consumption, 70% of the total petroleum consumption and 27% of the total greenhouse emissions [1]. A vital aspect of such effort is the investigation of the underlying chemical kinetics of combustion of various fuels which is critical for the development of alternative fuels as well as for the development of advanced combustion modes. A variety of

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experimental facilities such as flow reactors, combustion bombs, shock tubes and rapid compression (and expansion) machines (RCM/RCEM) have been in use for investigation of chemical kinetic aspects of combustion [2–4].

RCM/RCEM is an experimental facility used for investigation of combustion characteristics of various engine relevant fuels in low to intermediate temperature ranges. In an RCM/RCEM, a single shot, rapid compression of a test fuel can be studied in a well-defined and controlled environment without the complex fluid dynamics characteristic of a typical internal combustion engine [5,6]. The ability to retract the piston and perform an expansion stroke differentiates an RCEM from an RCM. While the gas pressure inside the combustion chamber constitutes the primary data, RCMs allow the flexibility to accommodate a wide variety of secondary investigation methods such as gas sampling for intermediate species identification [7–9], optical diagnostics [10–12], etc. This has led to the widespread use of RCM in chemical kinetic studies, especially the auto-ignition investigations of fuels at various temperature and pressure conditions for development, improvement and validation of the related chemical reaction mechanisms [13–20].

An inherent limitation of the autoignition investigation using conventional RCM comes from the extreme facility dependence of the thermodynamic path of compression, i.e. the pressure-temperature history during the compression process. The thermodynamic path of compression, for a given RCM, is a function of the piston trajectory and the heat transfer characteristics, which is generally fixed for a given operating point and is hardware dependent for the conventional RCM. Since the thermodynamic path of compression determines the degree of reaction progress during the compression, consequently, the intermediate species buildup at the end of compression, which is a function of thermodynamic path, is also heavily facility dependent. As a result, the facility-to-facility variability in heat transfer characteristics and the piston trajectory naturally translates into the facility-to-facility variability of thermodynamic path of compression, which manifests itself as facility-to-facility variability in the experimentally reported auto-ignition characteristics. This severely limits the reproducibility of experimental data reported by any facility. This problem has been well recognized and reported in the literature and more recently it has become a prevalent practice to supplement the auto-ignition experiment data with simulation results accounting for the facility specific thermodynamic path [5,6,9,21–23].

The controlled trajectory rapid compression and expansion machine developed at the University of Minnesota – Twin Cities addresses this limitations with the unique capability of precise control over piston trajectory. By changing the piston trajectory for compression (and expansion), the thermodynamic path of compression (and expansion) can be tailored as desired in the CT-RCEM. Besides, since the changes in the piston trajectory are made by digitally changing the reference motion profile sent to the controller, CT-RCEM allows a lower turnaround time, easier and smoother operation, a wider range, and, a higher resolution of the operating parameters.

A key novelty of the CT-RCEM, however, lies in its ability to allow the investigation of the dynamical relationship of the piston trajectory and the combustion characteristics. By suitable selection of piston trajectories, it is possible to attain (almost) similar thermodynamic state (pressure and temperature) at the end of compression (EOC) but with different thermodynamic path (pressure and temperature histories). This difference in the thermodynamic path can lead to a significant difference in the intermediate species concentration at the end of compression which can have a significant impact on the measured ignition delay. This extra degree of freedom facilitated by the CT-RCEM, provides, for the first time, a means to systematically obtain ignition delay measurement with different intermediate species buildup at EOC for a given thermodynamic state. To put this in perspective, for a given compression ratio (CR) the conventional RCM aim to achieve the shortest t_{50} or t_{50T} time – the duration of time for the final 50% rise in pressure or temperature, respectively – with the motivation to minimize the species buildup by the EOC [6]. However, using the CT-RCEM, it is possible to explicitly vary the t_{50} or t_{50T} for a constant CR, and to systematically account for its influence on the auto-ignition data. This constitutes a richer set of auto-ignition data from chemical mechanism development standpoint and enables a more stringent validation of the existing mechanisms.

Since the temperature measurement in an RCM is not straightforward, the temperature history is generally estimated from the pressure data, using a numerical model. While the computational fluid dynamics (CFD) based models are relatively the most accurate, the computational cost can be prohibitive even for relatively simple fuels. This has led to the widespread use of multi-zone models that are computationally tractable but can still provide reasonable accuracy. However, for CT-RCEM, the requirement of computational efficiency is even more pronounced. For an effective use of CT-RCEM, a numerical model is required to quickly predict, with reasonable accuracy, the evolution of the thermo-kinetic states in the combustion chamber for different piston trajectories. Analyzing the combustion characteristics for different trajectories through simulation allows the user to not only interpret the experimental results, but also to select the best suited trajectory, corresponding to a desired thermodynamic path, for a given experiment. High computational complexity of the model would make the analysis time prohibitive and reduce the overall turnaround time of the CT-RCEM. A physics based multi-zone model has been developed to meet the aforementioned requirements for the CT-RCEM.

In this study, we present, a systematic framework for the investigation of the effect of changing the piston trajectory – and hence, the thermodynamic path – on the combustion characteristics of fuels. This framework involves a concomitant use of the CT-RCEM and the proposed multizone model to leverage this extra degree of freedom. This allows us to obtain further insight into the chemical kinetics of combustion, especially the low temperature chemistry and auto-ignition dynamics. From application perspective, such insight is critical for enabling advanced combustion modes, such as HCCI, RCCI, etc. especially for renewable fuels [24,25]. Additionally, this capability makes the CT-RCEM naturally suitable for investigation pertaining to trajectory based combustion control [26–29].

In the following sections, we present the experimentally observed effect of changing thermodynamic path of compression on the auto-ignition of dimethyl-ether (DME), experimentally observed using the CT-RCEM, and explain these results in detail using the proposed model. We show that the changes in the shape of piston trajectory can have a significant impact on the ignition delay measurement. The change in the shape of piston trajectory has been realized, for this work, by changing the compression time for a constant CR. The study clearly shows a smaller compression time does not necessarily provide a smaller intermediate species buildup at the end of compression.

The rest of the paper is organized as follows. First, a brief description of the CT-RCEM is presented followed by the proposed multizone model. Next, the simulation results are benchmarked with non-reactive and reactive mixture tests to verify the fidelity of the model. After this, an investigation of the effect of piston trajectory on auto-ignition characteristics of dimethyl ether (DME) is presented. Ignition delay is measured for auto-ignition of DME: O_2: N_2 mixture (mole ratio 1:4:40 and 1:4:50) for same CR but different compression times, by changing piston trajectory in CT-RCEM. A reaction path analysis based on the simulation results from the model is presented next to interpret the experimental results. Finally, the importance of systematic evaluation of the thermodynamic path of compression corresponding to the piston trajectory is highlighted, followed by the conclusion.

2. Controlled trajectory rapid compression and expansion machine

A profound limitation of the conventional RCM/RCEM lies in the actuation philosophy which depends excessively on hardware