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Using rapid compression machines for chemical kinetics studies

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ABSTRACT

Rapid compression machines (RCMs) are used to simulate a single compression stroke of an internal combustion engine without some of the complicated swirl bowl geometry, cycle-to-cycle variation, residual gas, and other complications associated with engine operating conditions. RCMs are primarily used to measure ignition delay times as a function of temperature, pressure, and fuel/oxygen/diluent ratio; further they can be equipped with diagnostics to determine the temperature and flow fields inside the reaction chamber and to measure the concentrations of reactant, intermediate, and product species produced during combustion.

This paper first discusses the operational principles and design features of RCMs, including the use of creviced pistons, which is an important feature in order to suppress the boundary layer, preventing it from becoming entrained into the reaction chamber via a roll-up vortex. The paper then discusses methods by which experiments performed in RCMs are interpreted and simulated. Furthermore, differences in measured ignition delays from RCMs and shock tube facilities are discussed, with the apparent initial gross disagreement being explained by facility effects in both types of experiments. Finally, future directions for using RCMs in chemical kinetics studies are also discussed.

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1. Introduction

Rapid compression machines (RCMs) are considered an important experimental device for understanding low-to-intermediate temperature autoignition chemistry under idealized engine-like conditions. RCMs are able to interrogate the region responsible

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Review

for many of the fuel-specific effects during low-temperature combustion in engines, including combustion phenomena such as twostage ignition and the negative temperature coefficient (NTC) region of the ignition response. Although shock tubes are ideal for generating a homogenous high pressure and elevated temperature environment downstream of a reflected shock wave, the uniform conditions typically persist for less than 10 ms. Recent efforts, as discussed in Hanson and Davidson [1], have modified the driver section to extend shock tube use forignition delays of 50 ms and longer. Nevertheless, RCMs still hold the advantage in terms of capabilities that replicate reasonably well the low-temperature, high-pressure, and high fuel loading combustion conditions of reciprocating engines and gas turbines. In an RCM, experimental durations are longer than typically available in shock tubes. Therefore, an RCM gives accessibility to study autoignition chemistry at elevated pressure under conditions for which reactivity may be too slow for shock tubes. This typically involves temperatures in the range of 600-1100 K. The complementary combination of RCM and shock tube data has allowed the validation and refinement of various reaction mechanisms over a wide range of pressures and temperatures.

Like other experimental facilities, RCMs also have associated challenges. This paper first introduces the principle of RCM operation and then reviews the strengths and limitations of RCM facilities and results, with special emphasis on those aspects related to chemical kinetic model development and validation. In addition, major sources of errors, quantification of uncertainties, and issues for RCM experiments as well as representative RCM results and their complementary relation with shock tubes will be discussed. Note that this paper presents a succinct and informative review focusing on chemical kinetics studies using RCMs under homogenous conditions. An extensive review of RCM history and applications based on the outcome of the First International RCM Workshop [2] held at Argonne National Laboratory in August 2012 is currently in preparation by a group of workshop participants and will become available in the near future.

The history of compression machines for combustion studies can roughly be classified into three generations. First-generation compression machines were developed by Falk [3] and Dixon et al. [4,5] in which the fuel/oxidizer mixtures were continuously compressed using a piston driven by a falling weight or similar mechanism. The compression ratio in these first-generation machines was limited by the force required to oppose the reactor pressure to prevent piston rebound. The primary data obtained from the first-generation machines were ignition temperatures, while information about ignition delay was not available. After realizing the usefulness of ignition delays, second-generation compression machines were developed in which the reactor piston is held in a final position to create a constant volume reaction chamber. Cassel [6], Tizard and co-authors [7–9], Aubert [10], and Fenning and Cotton [11] thus developed compression machines capable of measuring ignition delay times. The first- and secondgeneration compression machines were limited primarily by the achievable compression ratio and long compression times, leading to the development of a third generation of compression machines. Very fast compression and higher compression ratios were the key features of this third generation compression machines, and thus they were referred to as Rapid Compression Machines. In the late 1960's Affleck and Thomas [12] developed a rapid compression machine using compressed gas driven piston assemblies. This permitted studies at higher compression ratios with associated shorter compression times of about 20 ms. Others RCMs developed by Carlier et al. [13], Griffiths et al. [14], Park at MIT [15], and by Mittal and Sung [16] used similar designs. In addition, a free-piston rapid compression facility was commissioned at the University of Michigan [17]. The high driving forces necessitate mechanisms to halt the piston at the end of the stroke. These mechanisms will be discussed in Section 2.1.

2. Operational principles and design features of RCMs

2.1. General considerations

An RCM simulates a single compression stroke of an engine, and is simple and relatively easy to operate. The fuel-oxidizer mixture introduced into the reaction chamber is rapidly compressed by a piston assembly in a process relatively close to adiabatic compression. The reactor piston is brought to rest and fixed in place at the end of compression. This rapid compression results in elevated temperature, high-pressure conditions in the reaction chamber, which can be used to investigate the autoignition characteristics (ignition delay time, heat release rate, etc.) of a given reactive mixture.

In an RCM experiment, the primary data consists of the pressure trace measured in the reaction chamber as a function of time during and after the compression. Typical pressure traces using non-reactive nitrogen and argon as test gases are shown in Fig. 1, demonstrating a rapid rise in pressure during the compression stroke followed by a gradual decrease in pressure due to heat loss from the constant volume reaction chamber at the end of compression. An overlap of four experiments for each test gas is shown in Fig. 1, where time zero is taken as the end of the compression stroke, when the pressure peaks. The operating conditions for the experiments are also indicated in Fig. 1.

Several important features related to RCM performance can be illustrated from these inert gas tests. It is seen in Fig. 1 that the overlapping pressure traces follow each other closely, indicating that highly repeatable experimental conditions are obtained, which is an important feature of RCM design. The RCM experiments depicted in Fig. 1, show that approximately 46% of the pressure rise occurs in the last 2 ms of the compression stroke. Such a rapid pressure rise is desirable in order to minimize the extent of chemical reaction during compression when using a reactive fuel mixture. However, the resulting pressure profile during the compression stroke strongly depends on the RCM's geometry, the machine design, and the operating condition. The data presented in Fig. 1 is taken from Ref. [16], which has a relatively fast (20 ms)



Fig. 1. Typical pressure traces for inert gas tests, demonstrating experimental repeatability. Subscripts: 0 - initial condition; C - condition at the end of compression; and ac - condition at the end of compression for a truly adiabatic compression. Truly adiabatic compression is calculated using the volumetric compression ratio; see Eq. (1).

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