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Interpretation of experimental data from rapid compression machines without creviced pistons

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ABSTRACT

Over the last two decades, experimental data of the nature of species evolution profiles and ignition delays from rapid compression machines (RCMs) has been used to develop and validate chemical kinetic mechanisms at low-to-intermediate temperatures and elevated pressures. A significant portion of this overall dataset is from RCMs that had not employed a creviced piston to contain the roll-up vortex. The detrimental influence of the roll-up vortex and the thermokinetic interactions due to the resulting temperature non-homogeneity during the negative temperature coefficient (ntc) regime have been documented in the literature. However, the adequacy of the homogeneous modeling of RCMs without creviced pistons during reactive conditions has not been investigated. In this work, computational fluid dynamics simulations of an RCM without a creviced piston are conducted for autoignition of *n*-heptane over the entire ntc regime over a range compressed pressures from 5 to 18 bar. The results from the CFD simulations highlight the non-homogeneity of autoignition and reveal significant quantitative discrepancy in comparison to homogeneous modeling, particularly for the hot ignition delay in the ntc regime. Specifically, the roll-up vortex induced temperature non-homogeneity leads to diminution of the ntc behavior. The experimental data from RCMs without creviced piston needs to be taken with caution for quantitative validation and refinement of kinetic mechanism, particularly at conditions when ntc behavior is highly pronounced.

1. Introduction

Experimental facilities for chemical kinetics studies are designed to minimize fluid dynamic effects, so that the chemistry can be isolated and studied with confidence. Over the last two decades considerable experimental data has been generated and used for chemical kinetics model development by using facilities such as shock tubes, flow reactors, rapid compression machines (RCMs), Jet-stirred reactors, and laminar flame experiments. Experimental data from such facilities can be very sensitive to experimental perturbations and non-idealities and researchers have continuously endeavored to minimize non-ideal effects and account for the unavoidable non-idealities by adequate modeling. For instance, it is now well recognized that the ignition in shock tubes at high pressures and low temperatures can be significantly influenced by fluid dynamic non-idealities as well as deflagrative processes typical of mild ignition [1]. Consequently, modeling strategies to satisfactorily account for such behavior have been developed and used successfully [1,2].

In regard to RCMs, it is well understood that the motion of the piston during the compression stroke creates a roll-up vortex that entrains the boundary layer into the core region [3–11]. In order to overcome this problem, crevices on the periphery of the pistons have been incorporated in RCMs, which successfully avoid the roll-up vortex, as demonstrated by experiments as well as CFD simulations [6,10,11]. However, a significant portion of the overall RCM dataset is from RCMs that had not employed a creviced piston to contain the vortex. Even though RCM researchers and kinetic modelers have acknowledged the effect of the vortex in RCMs without a creviced piston, the quantitative effect of the vortex on reactive experiments in such facilities has not been studied. On the other hand, such data continues to be widely used for validation and refinement of the latest kinetic mechanisms [12]. Therefore, it is important to understand the effect of the complicated fluid dynamics on the temperature field in these facilities, which thereby affects chemical reactions. The objective of the present work is to understand the same.

In this paper, CFD simulations for *n*-heptane ignition are conducted for an RCM without a creviced piston to understand the effect of fluid dynamics on autoignition. Further, homogeneous modeling of the CFD simulations is also conducted by using Senkin [13], while accounting for the compression and heat loss effects

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through adiabatic volume expansion [14]. Since homogeneous modeling is the only viable approach when detailed chemistry is considered and desired to be validated, a comparison of the CFD and homogenous modeling results is used to assess the suitability of the homogeneous modeling approach for RCMs without crevice pistons. In the following, computational specifications are provided, followed by the presentation and discussion of nonreactive and reactive CFD simulations as well as the comparison of the CFD and homogeneous modeling results. In addition, CFD results are also compared with experimental data.

2. Computational specifications

The RCM simulated here has a bore of 5 cm, compression stroke length of 19.9 cm and compression time of 60 ms. The compression ratio is kept fixed at 9.65. An RCM with these specifications has been extensively used over the last two decades and has provided admirable insights into the low temperature chemical kinetics of hydrocarbon fuels [e.g. 4,5,15,16]. CFD simulations are conducted for an axisymmetric configuration using the Ansys Fluent package [17]. Computations are performed from the beginning of the compression stroke. Initially, before the compression stroke begins, the gas mixture at rest is specified with a uniform temperature and known pressure. A fixed temperature and no-slip conditions are specified at the cylinder wall boundary and the piston surface. Simulations use the PISO (Pressure-Implicit Split-Operator) algorithm for the pressure–velocity coupling, the PRESTO (Pressure Staggering Option) scheme for pressure, and the second-order upwind discretization for density, momentum, and species.

During the compression stroke, a uniform piston velocity profile is specified except for an initial acceleration and deceleration at the end of compression of 1 ms each. Throughout the calculations, a time step of approximately 40 μs is taken, which was found to be adequate based on previous studies [14]. A typical computational grid distribution at the end of compression is shown in Fig. 1. In the axial and radial directions, finer grids are taken near the walls/surfaces. As reported previously [14], independence with respect to the size of the time-step and grid distribution were ascertained by checking selected calculations on a finer grid with smaller time-step size yielding identical pressure histories.

Adequate prediction of the temperature field is a prerequisite for capturing chemical processes and thermokinetic interactions during the induction period prior to autoignition. By comparing the CFD calculations with the experimental measurements, it was shown [11] that the laminar simulations perform much better than the turbulent simulations based on the Reynolds–Average–Navier Stokes equations in describing the temperature and velocity fields inside the RCM as well as post-compression heat loss. Therefore, all simulations are conducted for laminar flow conditions.

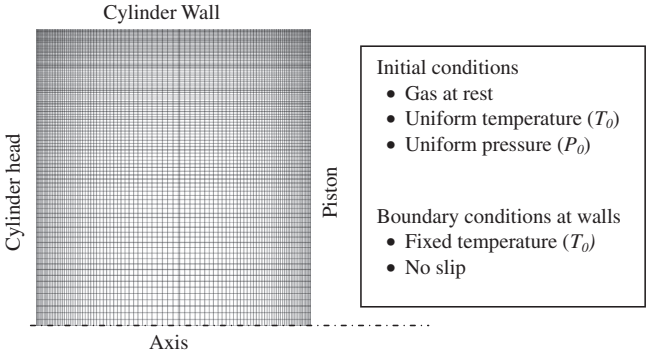

Fig. 1. Typical computational grid at the end of the compression stroke.

Table 1
Cases simulated: Molar compositions and pressure, temperature conditions.

Composition	Initial conditions at the start of compression		Pressure and temperature at the end of compression	
n-heptane/O_2/diluent	P_0 (bar)	T_0 (K)	P_C (bar)	T_C (K)
1/11/60	0.267	350	5.06–6.12	733–902
1/11/110	0.425	313	8.66–12	695–985
1/11/150	0.659	320	13.74–18.29	721–974

The kinetic mechanism of *n*-heptane and the associated thermodynamic and transport parameters are taken from the model of Liu et al. [18]. The skeletal mechanism of Liu et al. [18] consists of 43 species and 185 reactions. It has a concise representation of low-temperature kinetics, including formation of alkyl peroxy radicals, subsequent isomerization, and addition of second O_2. Furthermore, this skeletal mechanism was validated [18] against ignition delay measurements from RCM and shock tube at pressures up to 44 bar, species profiles for *n*-heptane oxidation in a plug flow reactor at 3 atm, and species distribution profiles in *n*-heptane-air counterflow diffusion flames.

In addition to the CFD simulations, homogeneous model simulations are conducted using Senkin [13]. As discussed in [14], the homogeneous calculations include the compression stroke and take the effect of heat loss during the compression and post-compression period into account through an approach based on volume expansion, which uses the empirically determined heat loss parameters obtained from the non-reactive pressure history. The volume expansion based approach assumes that there is 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 an adiabatic volume expansion and the 'effective volume' of the core region can be derived from the non-reactive pressure trace. The non-reactive pressure history is used as the reference to back calculate the time-dependent 'effective volume' of the core region. This approach has been previously validated for RCMs with optimized creviced pistons [14].

In this computational study, for every reactive CFD simulation, the corresponding non-reactive CFD simulation is conducted by suppressing the fuel oxidation chemistry during the calculations and the obtained pressure trace is used as the reference for deriving the 'effective volume' for the homogeneous simulation. The reactive CFD solutions are then compared with those obtained from the reactive homogeneous simulations using Senkin. As such, CFD calculations represent 'computational experiments', which are simulated through the homogeneous modeling. For homogeneous modeling of the RCM experiment, conditions specified in the Senkin calculations are those of a closed adiabatic system with the time-varying 'effective volume'.

Table 1 shows the compositions and pressure, temperature conditions for which simulations are conducted. The equivalence ratio for all compositions is 1, however higher dilution than air is used to avoid very short ignition delays. For a given dilution, the relative proportion of N_2 and Ar in the diluent is varied to change the compressed gas temperature while keeping the same initial temperature.