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Full Length Article

A comparison of sensitivity metrics for two-stage ignition behavior in rapid compression machines

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ABSTRACT

A rapid compression machine (RCM) multi-zone model is used to simulate the ignition of primary reference fuel (PRF) mixtures that exhibit two-stage ignition behavior. Sensitivity coefficients for each reaction in the PRF mechanism are calculated from four different metrics: (1) first-stage energy release, (2) first-stage pressure rise, (3) first-stage ignition delay time, and (4) total ignition delay time. The sensitivity coefficients are used to provide four unique rankings, and the rankings are compared using Spearman's rank correlation coefficient. Special emphasis is given to comparing the rankings based on first-stage energy release and total ignition delay time. The level of agreement between these two rankings is shown to depend on the reaction conditions. Simulation cases with high peak heat release rates during the first stage of ignition tend to exhibit disagreement in the rankings, indicating that new kinetic information can be obtained by studying first stage energy release in addition to total ignition delay time. Simulations show that the high peak heat release rates are associated with energy release across a broad range of temperatures (range can be in excess of 100 K even for lean conditions). This distribution leads to a discrepancy between sensitivity coefficients calculated for the total ignition delay time and the first-stage energy release. Sensitivity coefficients for the total ignition delay time are characterized by reactivity at the highest temperatures in the RCM, while sensitivity coefficients for the first-stage energy release are characterized by reactivity across the full range of temperatures in the RCM.

1. Introduction

Accurate kinetic models are an integral part of the workflow for improving combustion technology. By including these models within a larger reacting flow simulation, local rates of species formation and destruction and the corresponding energy release rates can be predicted. There is a widespread effort to validate and improve these models by conducting fundamental experiments under well-characterized conditions. Data from these experiments are compared with simulation predictions to assess the accuracy of a kinetic model, and when disagreement between the data and model exists, sensitivity analysis is frequently used to discern which reaction or set of reactions should be prioritized for improvement.

Rapid compression machine (RCM) experiments are one type of fundamental test used to validate kinetic mechanisms. The tests consist of measuring pressure during the ignition of a fuel-oxidizer mixture. The overall shape of the curve reflects the combined effects of chemical heat release, heat loss, crevice flow, and ringpack blowby. A model-based approach may be used to interpret these data to define an instantaneous heat release rate, but currently no such model implementation exists. Rather, the data are traditionally used to define one or more ignition delay times depending on whether the fuel exhibits single or two-stage ignition. These global metrics are used as the basis for conducting sensitivity analysis in RCM simulations.

The end use of kinetic models within engine computational fluid dynamics (CFD) codes requires they make accurate reaction rate predictions for widely varying in-cylinder conditions. It is important to consider that ignition delay data used to optimize kinetic mechanisms may not be sensitive to all the chemical pathways that are relevant to energy release within the engine cylinder, which is especially relevant for modeling apparent heat release rates calculated from engine data. This paper considers the definition of two additional metrics that can be used with RCM experiments to investigate the roles of these reactions for two-stage ignition fuels. These metrics are the total first stage energy release (ΔH_1) and the total pressure rise during the first stage of ignition (ΔP_1). The authors hypothesize that these metrics will be sensitive

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to the full distribution of temperatures within the RCM, and therefore sensitive to a set of reactions that may be unique from the controlling chemistry for the first stage and total ignition delay times. ΔH_1 is proposed for study because it is a proxy to directly validating heat release rate in the RCM, and ΔP_1 is proposed because it can be easily calculated from pressure data obtained during a RCM experiment. Although ΔH_1 can be calculated from RCM data, its accuracy is highly dependent on the rigor of the model used to interpret the pressure data. To determine the value of ΔH_1 and ΔP_1 as validation metrics, this paper presents sensitivity analysis with respect to the four metrics of ΔH_1, ΔP_1, τ (total ignition delay time) and τ_1 (first stage ignition delay time). The results are analyzed to identify the important chemical reactions for governing these phenomena.

For fuels/tests that exhibit two-stage ignition, RCM experiments show that the hot ignition timing is influenced by the energy released during the first stage of ignition. Experiments reported by Tanaka et al. [1] showed that as the pressure rise due to first stage ignition increased, the total ignition delay time decreased. Tanaka et al. indicate this occurs because increases in pressure rise due to first stage activity correspond to higher gas temperatures that accelerate the onset of hot ignition. This is consistent with the interpretation of Ribaucour et al. [2] and later reaffirmed by Westbrook [3], that the onset of hot ignition is controlled by a critical temperature at which H_2O_2 decomposes rapidly. The time at which a mixture reaches this condition in a RCM experiment was shown to depend on the timing and magnitude of energy release in the first stage of ignition. Additional studies in the literature demonstrate the dependence of first stage energy release on the reaction conditions. The simulations of Zhao and Law [5] quantified the influence of equivalence ratio and reaction temperature (*i.e.*, the "compressed temperature" in RCM experiments) on the first stage temperature rise and therefore the total ignition delay time. Zhang et al. [4] quantified the role of unique factors influencing negative temperature coefficient behavior (NTC), showing that the temperature rise due to first stage energy release plays a substantial role in determining the total ignition delay time. Given the evidence from these prior works, reactions that strongly influence τ_1 and ΔH_1 (or ΔP_1) should also strongly influence τ. There is limited data in the literature to support this view, however, because the majority of sensitivity analyses use a sensitivity metric based on τ alone, with τ_1 being neglected. Some exceptions to this include the dimethyl ether study (DME) by Mittal et al. [6] and the gasoline surrogate works of Kukkadapu et al. [7,8]. In their study of DME ignition behavior, Mittal et al. reported that the most influential reaction for both τ_1 and τ was the isomerization of the methoxymethyl-peroxy radical [6]. However, inspection of their results suggests a difference in ranking for other reactions. Kukkadapu et al. [5] calculated sensitivity coefficients for τ_1 and τ in the low-temperature, lean-to-stoichiometric region using an adiabatic, constant volume simulation. The analysis was based on a brute force method and considered a four-component surrogate of iso-octane, *n*-heptane, toluene, and 2-pentene. The largest sensitivity coefficients for τ_1 were associated with H-atom abstraction reactions by OH from parent fuel molecules (namely *n*-heptane and iso-octane) and isomerization reactions of heptylhydroperoxy radicals. These same reaction classes were also influential for the total ignition delay time, further supporting the dependence of τ on τ_1. A relationship between τ and τ_1 is clearly supported by these studies, but the relationship is not well characterized as it is often based on analysis at only one or a few conditions.

The main objective of this paper is to compare and contrast the governing chemistries for the RCM validation metrics of ΔH_1, ΔP_1, τ, and τ_1 for a variety of test conditions. The basic approach used is to conduct brute force sensitivity analysis on the metrics for a wide range of RCM simulation cases. By understanding these metrics and their sensitivities, RCM experiments may be optimally designed to probe a reaction or reaction set of interest. This will enable more comprehensive analysis of RCM data that can be used to improve kinetic models.

2. Methods

2.1. Modeling approach

To rigorously characterize the reaction sensitivities at a given test condition, all of the important reactor physics must be modeled. This is accomplished in this work by use of a multi-zone model (MZM) designed to simulate the heat loss, crevice flow, and chemical energy release during an RCM experiment [9,10]. The model divides the main reaction chamber into a set of concentric zones, each with a characteristic temperature and composition that evolves during the simulation. The zones communicate with one another by conduction only, as there is no mass transfer between the zones. The influence of the crevice and ringpack flows on the main chamber conditions are also modeled, assuming quasi-steady flow through the tapered gap that connects the crevice to the main chamber. The model is implemented in Python Cantera, and has been validated to yield cylinder-averaged speciation predictions within 15% of those predicted by computational fluid dynamics (CFD) [9]. All simulations were conduced with 15 zones in the main reaction chamber, and the simulations were terminated upon reaching an average cylinder temperature of 1200 K. The RCM modeled in this paper has an 8 inch stroke and a 2 inch bore. A single arbitrary velocity profile was used for all of the simulations, with a compression time of 32 ms. Depending on the compression ratio for a given simulation case, the modeled RCM piston has a crevice volume between 9% and 13% of the reaction chamber volume at top dead center (TDC). Use of the MZM for this study is very important because reliable predictions of the RCM sensitivity metrics ΔH_1, ΔP_1, and τ cannot be obtained during multi-stage ignition events using constant volume or effective volume modeling techniques [11]. The ΔH_1 and ΔP_1 metrics are particularly sensitive to the temperature distribution in the RCM, thus single zone models are inadequate for conducting the sensitivity analysis presented in this work. In fact, modeling the RCM reactor physics is critical to this work because they strongly influence our observations of ignition behavior. It is noted that ΔH_1 is used in this study as a metric because it serves as a proxy to the temperature increase during first stage ignition. Section 1 describes how the temperature increase due to first stage ignition is important for determining the hot ignition timing, and this increase is driven by ΔH_1.

The PRF mechanism of Tsurushima [12] is used in this work primarily because it is compact (33 species and 38 reactions), and because it is capable of modeling two-stage ignition behavior. The model was developed using the PRF mechanism of Tanaka et al. [13] as a baseline, and it has been validated with shock tube ignition delay data in the temperature range of 700–1200 K and the pressure range of 6–42 bar. However, given that the objective is to characterize reaction sensitivities with respect to ignition phenomenology, the predictive accuracy of the mechanism is of reduced importance. It would be preferable to conduct this investigation with a detailed mechanism, but this would be impractical due to the computational burden of simulating fuels that exhibit two-stage ignition.

2.2. Analysis procedure for simulation results

The MZM is used in this work to simulate all of the test cases described in the following section. Sample simulation output for