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Computational characterization of ignition regimes in a syngas/air mixture with temperature fluctuations

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Abstract

Auto-ignition characteristics of compositionally homogeneous reactant mixtures in the presence of thermal non-uniformities and turbulent velocity fluctuations were computationally investigated. The main objectives were to quantify the observed ignition characteristics and numerically validate the theory of the turbulent ignition regime diagram recently proposed by Im et al. 2015 [29] that provides a framework to predict ignition behavior *a priori* based on the thermo-chemical properties of the reactant mixture and initial flow and scalar field conditions. Ignition regimes were classified into three categories: *weak* (where deflagration is the dominant mode of fuel consumption), *reaction-dominant strong,* and *mixing-dominant strong* (where volumetric ignition is the dominant mode of fuel consumption). Two-dimensional (2D) direct numerical simulations (DNS) of auto-ignition in a lean syngas/air mixture with uniform mixture composition at high-pressure, low-temperature conditions were performed in a fixed volume. The initial conditions considered two-dimensional isotropic velocity spectrums, temperature fluctuations and localized thermal hot spots. A number of parametric test cases, by varying the characteristic turbulent Damköhler and Reynolds numbers, were investigated. The evolution of the auto-ignition phenomena, pressure rise, and heat release rate were analyzed. In addition, combustion mode analysis based on front propagation speed and computational singular perturbation (CSP) was applied to characterize the auto-ignition phenomena. All results supported that the observed ignition behaviors were consistent with the expected ignition regimes predicted by the theory of the regime diagram. This work provides new high-fidelity data on syngas ignition characteristics over a broad range of conditions and demonstrates that the regime diagram serves as a predictive guidance in the

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understanding of various physical and chemical mechanisms controlling auto-ignition in thermally inhomogeneous and compositionally homogeneous turbulent reacting flows.

Keywords: Direct numerical simulation; Strong and weak ignition; Ignition regimes; Temperature fluctuations; Computational singular perturbation

1. Introduction

Low-temperature combustion (LTC) strategies have the potential to improve efficiency and reduce NO_x emissions in both transportation [1] and stationary power devices [2]. Reductions in combustion temperature can be achieved by operating at lean, nearly homogeneous, and/or diluted, conditions. However, issues related to combustion stability, safety and control may arise at these conditions, due to increased influence of abnormal ignition behaviors such as early ignition and flashback in gas turbines [2,3] or knock in reciprocating engines [4]. Improved understanding and better prediction of auto-ignition characteristics are therefore valuable for successful implementation of these advanced technologies.

Many experimental studies have been conducted to investigate auto-ignition of different fuels such as hydrogen [5–9], iso-octane [10,11] and syngas [12,13], at conditions relevant to practical combustion systems. Two types of auto-ignition regimes were commonly observed: strong (spatially homogeneous ignition) and weak (localized reaction sites and deflagration). Moreover, the boundary between strong and weak ignition regimes, known as the *strong ignition limit*, was found to coincide with an iso-line of the sensitivity of homogeneous ignition delay time to temperature, $d\tau_{ig}/dT$, in the pressure-temperature space [6,13]. Recent experimental investigations of syngas auto-ignition [14–18] at conditions relevant to gas turbine operation reported large discrepancies between measurements and homogeneous chemical kinetic modeling predictions of ignition delay times, with the former being orders of magnitude lower than the latter. Mansfield and Wooldridge [13] studied syngas auto-ignition in a rapid compression facility and demonstrated that the discrepancy was due to transition from strong to weak ignition regime as the initial mean temperature was lowered. In addition, a simple criterion proposed by Sankaran et al. [19] (referred to as the Sankaran criterion here), based on Zel'dovich's original theory [20] was found to capture the experimentally observed strong ignition limit *a priori*. This predictive criterion is defined as the ratio of laminar flame speed to the thermal gradient driven spontaneous propagation speed. Pal et al. [21] further numerically validated the Sankaran criterion as a predictive indicator of the ignition regime for homogeneous mixtures in the presence of thermal non-uniformities through parametric studies of syngas auto-ignition in a one-dimensional configuration.

In addition to thermal inhomogeneities, the presence of turbulence may also significantly influence auto-ignition phenomena in practical devices. Ihme and co-workers [22,23] demonstrated using a reduced order modeling approach that turbulent fluctuations could result in significant advancement of overall ignition. A number of DNS studies [24–28] have revealed that thermal stratification and turbulence can influence auto-ignition phenomena in LTC engines. More recently, Im et al. [29] conducted a theoretical scaling analysis and proposed non-dimensional criteria in terms of the characteristic Damköhler and Reynolds numbers of a system to predict the occurrence of strong and weak ignition regimes in thermally inhomogeneous turbulent reacting flows. The criteria formulated by extending the original Sankaran criterion [19] and taking into account the effects of passive scalar mixing due to turbulence, ultimately led to the development of a turbulent ignition regime diagram [29]. An alternative version of ignition regime diagram has also been proposed by Grogan et al. [30].

The present computational study investigates the effects of thermal inhomogeneities and turbulence on syngas auto-ignition behavior. 2D DNS of auto-ignition in a lean syngas/air mixture are performed at various parametric conditions. The high-fidelity simulations aim to provide additional insight into the range of ignition behaviors that can be expected under high-pressure low-temperature conditions, and also provide numerical validation of the turbulent ignition regime diagram [29]. In the next section, the ignition regime diagram is briefly reviewed. The numerical setup for simulations is presented next. The auto-ignition behaviors are subsequently characterized and the results are discussed in the context of the corresponding predictions of the regime diagram.

2. Turbulent ignition regime diagram

One of the non-dimensional parameters used as an ignition regime criterion is the Sankaran

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