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Experimental and numerical investigation of hetero-/homogeneous combustion-based HCCI of methane–air mixtures in free-piston micro-engines

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ABSTRACT

The hetero-/homogenous combustion-based HCCI (homogeneous charge compression ignition) of fuel–lean methane–air mixtures over alumina-supported platinum catalysts was investigated experimentally and numerically in free-piston micro-engines without ignition sources. Single-shot experiments were carried out in the purely homogeneous and coupled hetero-/homogeneous combustion modes, involved temperature measurements, capturing the visible combustion image sequences, exhaust gas analysis, and the physicochemical characterization of catalysts. Simulations were performed with a two-dimensional transient model that includes detailed hetero-/homogeneous chemistry and transport, leakage, and free-piston motion to gain physical insight and to explore the hetero-/homogeneous combustion characteristics. The micro-engine performance concerning combustion efficiency, mass loss, energy density, and free-piston dynamics was investigated. The results reveal that both purely homogeneous and coupled hetero-/homogeneous combustion of methane–air mixtures in a narrow cylinder with a diameter of 3 mm and a height of approximately 0.3 mm are possible. The coupled hetero-/homogeneous mode can not only significantly improve the combustion efficiency, in-cylinder temperature and pressure, output power and energy density, but also reduce the mass loss because of its lower compression ratio and less time spent around TDC (top dead center) and during the expansion stroke, indicating that this coupled mode is a promising combustion scheme for micro-engine. Heat losses result in higher mass losses. Heterogeneous reactions cause earlier ignition, which is very favorable for the micro-device.

1. Introduction

Recently, micro-scale combustion has attracted increased attention because of the growing interest in developing portable power generation systems, with increasing efforts toward miniaturizing thermal engines for electricity production of a few tens of Watts [1]. Specifically, the high energy density of hydrocarbon fuels allows for the realization of micro-scale power generation systems [2]. Among the micro-scale system using the chemical energy of hydrocarbon fuels, micro-scale heat engine is being explored [3]. Micro-engine-based power supplies can deliver large energy density, and may eventually replace traditional lithium-ion batteries in various applications [4].

How to prevent thermal and radical quenching and achieve stable combustion is one of the most challenging issues to the micro-engine designer. Quenching is a matter of great concern because the specific heat transfer rate varies inversely with the characteristic dimension of the combustion chamber [5]. As engine size decreases, the surface-to-volume ratio increases, resulting in increased heat losses and increased potential destructions of active radicals on the combustion chamber walls. These mechanisms will increase the chemical reaction time and possibly inhibit the onset of homogeneous ignition, resulting in thermal or radical quenching [6]. Another concern is residence time, decreasing the dimension of the combustion chamber results in significant reduction of residence time because the flow velocity cannot be reduced accordingly. Insufficient residence time results in partial or incomplete combustion, in turn resulting in insufficient heat generation and further quenching [7]. In micro-scales, traditional engine combustion schemes are generally infeasible because of quenching effects and insufficient residence times. When considering micro-scale application, HCCI combustion mode is a promising alternative because it has the following experimentally verified characteristics: ignition is not initiated by an external event; the charge is

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consumed very rapidly; ignition occurs simultaneously at numerous locations inside the combustion chamber; and an absence of traditional flame propagation [8]. In the context of micro-combustion, the fundamental attributes of HCCI combustion are that an external ignition system is not required, and that the charge is combusted essentially without flame propagation. In addition, auto-ignition suggests that the charge is consumed both uniformly and rapidly, consequently minimizing quenching effects and without resorting to complicated ignition schemes. This concept may be a way toward elimination of ignition sources from micro-scale devices, resulting in further reduction of system size [9]. Additionally, HCCI combustion rate limited by chemical kinetics rather than transport and essentially no flame propagation result in shorter charge consumption time and in turn higher engine speed and efficiency [10]. These traits essentially bring HCCI combustion closer to a constant volume procedure, pushing the thermodynamic process closer to an ideal Otto cycle [11]. Furthermore, the ability to sustain homogeneous combustion with very lean mixtures reduces fuel mass losses through the leakage between the cylinder and piston, adversely enhancing fuel consumption efficiency [10,11].

However, HCCI engines are more difficult to control than traditional engines. The combustion occurrence (or ignition) depends on chemical kinetics and the compression process [12,13]. Therefore, controlling ignition timing is a challenge because it must be done indirectly. Experiments have demonstrated that employing a variable compression ratio is a promising approach to control HCCI ignition [9]. Therefore, to utilize this strategy, an untraditional engine such as a free-piston engine (FPE) is necessary, and is a very promising HCCI engine concept due to its valuable feature of variable compression ratio. The distinguishing feature of this device is a mechanically unconstrained free-piston; the free-piston motion is not restricted by a crankshaft mechanism, but is completely determined by gas pressure forces. In addition, the free-piston engine is a promising power generation device, offering the benefits of higher thermal efficiency and heat release rate compared to those of the traditional engine [14], extensive operation optimization [15], mechanical simplicity [16], multi-fuel/combustion mode flexibility [17], and reduced NO_x formation [18,19].

Computational models for simulating combustion and heat transfer of HCCI engines require detailed chemistry models; this is primarily because the ignition of HCCI engines is more sensitive to chemical kinetics. In addition, computational models have demonstrated that the importance of accounting for the fact that the in-cylinder mixture is actually in-homogeneous, particularly in terms of temperature field [20]. This in-homogeneity is driven by heat transfer from the combustion chamber walls and the turbulent mixing of fuel. Moreover, recent simulations have demonstrated that the charge inhomogeneity has a significant effect on the pressure rise rates and the consequential engine performance [21,22]. The charge in-homogeneity would increase with decreasing cylinder size because in-homogeneities in the cylinder is caused by the thermal boundary layer adjacent to the cylinder walls (e.g., the in-homogeneity in the temperature field is caused by the mixing of the colder gases in the boundary layer into the bulk gas) [20]. The increased charge in-homogeneity, coupled with the high surface-area-to-volume ratio, may ultimately constrain the combustion chamber dimension. Furthermore, homogeneous combustion is mainly controlled by the temperature boundary layer and reactant species profiles [23,24]. Consequently, in this work, a spatial dimensionality of at least two is necessary to correctly describe interphase transport and homogeneous combustion in particular.

Additionally, HCCI suffers from comparatively large hydrocarbon and carbon monoxide emissions, and especially from poor power density [25,26]. When considering micro-scale application, however, HCCI is pursued because the charge can be consumed rapidly, and especially be ignited without additional ignition devices. Furthermore, although purely homogeneous combustion can be stabilized in micro-scales [27,28], coupled hetero-/homogeneous combustion is the preferred route because of large surface-to-volume ratio issues, compared to purely homogeneous combustion [29,30]. Heterogeneous reaction broadens the classical flammability limits [31], and results in stable combustion even in the presence of high heat losses [32,33]. Coupled hetero-/homogeneous combustion becomes an attractive technology with prototype meso-scale devices (miniature free-piston Stirling engine) already successfully demonstrated [34]. Recent works [35,36] have further demonstrated the potential of catalytically-coated walls in inhibiting intrinsic flame instabilities.

The coupled hetero-/homogeneous combustion methodology crucially depends upon multidimensional CFD (computational fluid dynamics) modeling needed for combustor design [2,24,29,30], as well as upon advances in catalyst preparation technology (development of active and thermally stable catalysts) [32,35,37]. Nowadays, in the context of micro-combustion, two-dimensional models with detailed hetero-/homogeneous chemistry [37–40] have become common study methods for steady simulations. However, to the best of our knowledge, CFD modeling based on such detailed chemistry have not been applied to time-accurate transient simulations, coupled with HCCI and dynamic mesh. Transient catalytic channel simulations with detailed hetero-/homogeneous chemistry were reported in previous work [2,41–43] using a commercial CFD software; however, these studies did not address issues such as compression ignition (or HCCI), leakage, free-piston movement, turbulent transport, and hetero-/homogeneous chemistry coupling. In addition, although the heterogeneous catalytic oxidation and the free-piston HCCI engine have been widely studied by means of experimental and numerical methodologies [2,5,6,8,9,17,24,29,30,32,35,37,44,45], fundamental studies focused on hetero-/homogeneous combustion in free-piston micro-engines are still lacking and require further investigation.

The present work undertakes a combined experimental and numerical investigation of the hetero-/homogenous combustion-based HCCI of fuel–lean methane–air mixtures over alumina-supported platinum catalysts in a free-piston micro-engine, which is candidate for small portable power generation applications. Single-shot experiments in the purely homogeneous and coupled hetero-/homogeneous combustion modes were performed in a free-piston micro-engine with a cylinder bore of 3 mm, involved temperature measurements, capturing the visible hetero-/homogeneous combustions image sequences, exhaust gas analysis, and physicochemical characterization of catalysts. A two-dimensional transient numerical model incorporating detailed hetero-/homogeneous chemistry and transport, leakage, dynamic mesh, turbulence, and thermodynamic–dynamic balance is developed to interpret the single-shot experimental results as well as to explore hetero-/homogenous combustion characteristics. Following numerical validation and interpretation of the single-shot experimental results, the transient model was used to investigate the purely homogeneous and coupled hetero-/homogeneous combustion characteristics. In addition, the performance of free-piston micro-engines with regard to fuel conversion efficiency and mass loss was investigated. The primary objective of this work is to explore the feasibility of coupled hetero-/homogeneous combustion-based HCCI in free-piston micro-engines, and to characterize the purely homogeneous and coupled hetero-/homogeneous combustion at the micro-scale as well as to explore the free-piston dynamics. Of particular interest in the present work is to resolve the poor power density and low fuel conversion