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Detonation behaviors of syngas-oxygen in round and square tubes

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ABSTRACT

The present study reports the detonation behaviors of syngas-oxygen mixtures in three 2 m long tubes, including two circular tubes ($D = 32$ mm and 18.5 mm, D is the inner diameter) and a square tube ($H = 32$ mm, H is the inner side). Three stoichiometric syngas-oxygen mixtures, i.e., $\text{CO} + \text{H}_2 + \text{O}_2$, $2\text{CO} + \text{H}_2 + 1.5\text{O}_2$, $3\text{CO} + \text{H}_2 + 2\text{O}_2$ were used. Evenly spaced photodiodes were used to determine the detonation velocity while the soot foil technique was adopted to record the cellular structure. The results indicate that well within the limits, the detonation propagates at a steady velocity close to the Chapman-Jouguet value. The velocity deficits are more prominent at decreased initial pressure (equivalently, larger cell size and less sensitivity). At the limiting pressure, the velocity deficits of three mixtures in various tubes are approximate 14%–17%. The experimental velocity deficits were compared with a modified model based on Fay's theory, in which the cell size as well as the corresponding cell length are measured. The experimental velocity deficit is in excellent agreement with the theoretical prediction. The effective diameter, D_e , rather than the hydraulic diameter, is found to be a more appropriate parameter for the characterization of the detonation velocity in both round and square tubes. Further, a linear correlation between the normalized detonation velocity and $(D_e \cdot p_0)^{-1}$ is observed. The cellular structure shows that the single-headed spin occurs in all tubes when the detonation limits are approached.

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Introduction

Synthetic gas (syngas) fuels are particularly promising in IGCC (integrated gasification combined cycle) due to the rich

sources, low pollution emissions and high energy conversion efficiencies [1,2], which can be extracted from solid fuels (e.g., coal, biomass) or liquid fuels. Depending upon the fuel source and the refining process, the constituents of syngas may be

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various [3]. Hydrogen and carbon monoxide are typically the primary components, and methane or inert gases (e.g., N₂, CO₂ and H₂O) may be the subordinate compositions [3–5]. Table 1 shows some fundamental combustion parameters of hydrogen, carbon monoxide and methane in air/oxygen [3,6]. One can see that both hydrogen and carbon monoxide have broad flammable ranges. Therefore, safety problems related to the syngas still persist in view of the existence of hydrogen and carbon monoxide. Carbon monoxide is a toxic and flammable gas, the density of which is consistent with that of air. In spite of the extremely buoyant of hydrogen, syngas leakage in a confined space is still very dangerous [7,8]. Once the flammable vapor cloud is ignited accidentally, a deflagration may be generated. Further, if the flame encounters practical obstacles or cavities, the deflagration to detonation transition (DDT) or even the worst scenario, a detonation may occur, causing tremendous disasters [9–11]. Thus, it is of importance to study the detonation characteristics of syngas.

Previous investigations related syngas are most focused on the explosion parameter (e.g., explosion limit, burning rate, laminar burning velocity and explosion pressure, etc.) [1,2,8,12–15]. However, the detonation dynamic parameters (detonation limits, detonation cell size, critical tube diameter, critical energy for direct detonation initiation) [16] of syngas are fairly lacking, which are needed to be given full consideration. The detonation limit is one of the most fundamental dynamic parameters for hazard assessment, and outside the limit a detonation cannot be self-sustained [17]. In recent years, numerous investigations have been performed to study the detonation limits of hydrocarbon fuels and hydrogen in various ducts [17–30]. It is shown that well within the limits, the detonation velocity is very closed to the theoretical Chapman-Jouguet (CJ) detonation velocity. As the limits are approached, the velocity deviates from the CJ value. Various factors, e.g., heat and momentum losses, flow divergence rooted in the boundary layer effect and the interference of the wall with detonation instability, can be responsible for the velocity deficit [22]. The propagation mechanisms of the cellular detonation are very complex near the limits and no completely quantitative theory for the prediction of the limits is available up to date [19]. However, the behaviors of the

detonation near the limits are almost uniform, i.e., rapid velocity decrease, increased velocity fluctuation and increased cell size. In a smooth tube, as reported by Haloua et al. [31], depending upon the initial conditions (e.g., mixture stability, tube geometry), the detonation modes near the limits can be stable (spinning) detonation, unstable (galloping and stuttering) detonation and fast flame. Lee [32] indicated that the unstable detonations near the limits are generally formed in unstable mixtures in small diameter tubes. Thus, the onset of single-headed spin could be considered as the universal limiting condition. In a square channel, the detonation limits were also found to correspond to the single-headed mode [33,34].

Another important dynamic parameter is the detonation cell size (also known as the transverse wave spacing), λ , which is intimately associated with the other dynamic parameters [16]. For example, the detonation limits are often correlated with $\lambda = C$ in a smooth duct, where C is the perimeter of the cross-section [19,22]. Long foils coated with uniform carbon soot are often used to record the cellular structure of the detonation front. As argued by Ng [35], the cellular structure is characterized by the activation energy and chemical reaction. The stability and sensitivity of a given mixture can be reflected by the “fish-scale” pattern. More specifically, the stability is high for regular cellular structure while more sensitive the mixture is for decreased cell size.

In this study, the detonation behaviors of stoichiometric syngas-oxygen mixtures were investigated systematically in tubes with various cross-sections (circular and square). Three fuel mixtures were used: 25%H₂+75%CO, 33.3%H₂+66.7%CO and 50%H₂+50%CO ([CO]/[H₂] = 3, 2, 1). Photodiodes and soot foils were employed to obtain the detonation velocity and the cell structure, respectively. The cell size was measured based on the soot imprint. The experimental velocity deficits were analyzed and compared with the theoretical calculation using Fay's model [36]. Lastly, the cellular structures near the limits were studied.

Table 1 – Some explosion-related properties of hydrogen, carbon monoxide and methane in air/oxygen [3,6].

Component	Hydrogen	Carbon monoxide	Methane
Flammability limits (vol%), minimum ignition energy (MIE, mJ), auto-ignition temperature (AIT, °C) and maximum experimental safe gap (MESG, mm) of vapors in air			
Lower limit	4.0	12.5	5.0
Upper limit	75.0	74.0	15.0
MIE	0.017	–0.30	0.30
AIT	520	610	630
MESG	0.20	0.91	1.14
Flammability limits (vol%), minimum ignition energy (MIE, mJ), auto-ignition temperature (AIT, °C) of vapors in oxygen			
Lower limit	4.0	12.5	5.0
Upper limit	94.0	94.0	61.0
MIE	0.0012	–	0.003
AIT	400	590	555

Experimental details

Fig. 1 shows the experimental setup used in this study. The stainless steel detonation tube consists of two sections, i.e., the driver section and the test section. The driver section is a 3300 mm long, 48 mm inner-diameter tube. A 1.5 m Shchelkin spiral was placed near the beginning of the driver section to facilitate the rapid formation of detonations. Three 2000 mm long tubes were used as the test sections, i.e., two round tubes with the inner-diameters (D) of 32 mm (RT₁) and 18.5 mm (RT₂), and a 32 mm inner-side (H) square tube (ST).

Three stoichiometric combustion mixtures of CO+H₂+O₂, 2CO+H₂+1.5O₂ and 3CO+H₂+2O₂ were used as the test gases. The mixtures were mixed in a cylinder vessel for 24 h, which could ensure the homogeneity. All experiments were performed at room temperature (298 K). The initial pressures in both the mixing vessel and the tube were monitored by an absolute digital manometer (SXT-4A, 0–150 kPa) with an accuracy of ± 0.1 kPa. The ignition was achieved by two copper electrodes connected to a high voltage discharger. Eleven

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