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Influences of different diluents on ignition delay of syngas at gas turbine conditions: A numerical study☆

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ABSTRACT

Ignition delay of syngas is an important factor that affects stable operation of combustor and adding diluents to syngas can reduce NO_x emission. This paper used H_2O, CO_2 and N_2 as diluents and calculated ignition delay of syngas in temperature range of 900–1400 K and at pressures of 10 and 30 atm respectively. In high temperature range, comparing with N_2 dilution, adding H_2O and CO_2 can significantly inhibit autoignition of syngas because they have higher collision efficiencies in reaction $H + O_2 (+M) = HO_2 (+M)$. As for low temperature conditions, adding H_2O can increase reactivity of syngas, especially under high pressure, because of its high collision efficiency in reaction $H_2O_2 (+M) = 2OH (+M)$. Comparing with different dilution rates shows that for syngas and operating conditions in this paper, adding N_2 mainly influences temperature rising process of syngas combustion, thus inhibiting reactivity of syngas. In addition, this paper calculated ignition delay of syngas at different equivalence ratios ($\varphi = 0.5, 1.0$). Higher equivalence ratio ($\varphi \le 1$) means that less air (especially N_2) needs to be heated, thus promoting ignition of syngas.

1. Introduction

Syngas (main compositions are H_2 and CO) has drawn more and more attention recently because of its higher efficiency and clean property used in integrated gasification combined cycle (IGCC). However, syngas, especially with higher hydrogen content, has shorter ignition delay time and is easy to ignite automatically, which affects safe operation of gas turbine. So it's necessary to research influences on ignition delay of syngas with various diluents and provide references for actual combustor design.

Generally, ignition delay of fuel is measured by shock tube [1–5] and rapid compression machine (RCM) [6,7]. Shock tube is usually used to measure ignition delay under high temperature and ignition time is defined as the time between arrive of reflected shock ware and maximum OH^* gradient. Thi *et al.* [1] researched ignition delay of multi-component syngas mixtures and they have illustrated the effect of equivalence ratio. And ignition of lean CO/H_2 in air was conducted by Kalitan *et al.* [3] at $T = 890$–1300 K and $p = 0.1, 0.25$ and 1.5 MPa. Ignition delay measured by RCM is defined as the period between end of compression and maximum pressure gradient in ignition process. Mansfield and Wooldridge [6] measured ignition delay of syngas at high pressure and low temperature conditions. And Walton *et al.* [7] performed ignition of syngas at gas turbine conditions. In general, data measuring process costs lots of time and efforts. In addition, actual syngas compositions used in IGCC as well as operating conditions may not be exactly consistent with experimental measurements.

Kinetic simulation is an important way to calculate ignition delay of fuels [8,9]. Using relevant H_2/CO reaction mechanisms [10–13], ignition delay of syngas can be simply calculated at different temperatures and pressures with various compositions in syngas, which helps to save time as well as experimental cost and provide references to practical designing of combustor. Based on GRI Mech3.0 [10] and considering the rate coefficient of $H + O_2 (+M) = HO_2 (+M)$ and third body efficiencies published recently, Davis *et al.* [11] put forward a H_2/CO combustion mechanism (Davis Mech) which included 14 species and 30 elementary reactions to simulate high-temperature H_2 and CO combustion and they compared calculated ignition delay, laminar flame speed and extinction strain rate with experimental results. Petrova and Williams [12] presented a simplified hydrocarbon reaction mechanism (SD Mech) which contains 21 steps among 8 species for H_2 combustion, 30 steps among 11 species for CO combustion, and more than 300 steps for other hydrocarbon combustion which means it takes long time for CO/H_2 combustion calculation. Kéromnès *et al.* [13] presented a H_2/CO reaction mechanism (NUIG Mech), and further validation was made at different H_2/CO molar ratios, pressures and equivalence ratios. In addition, 10 steps of OH^* Chemiluminescence reaction were added in this mechanism. Besides, accuracy of these reaction mechanisms has drawn more and more attention. Fischer and Jiang [14–16] put forward a numerical optimization method for

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mechanism evaluation and they have checked the accuracy of several published mechanisms for combustion of biogas and bio-syngas.

Research of lean premixed combustion shows that lowering maximum temperature in combustion process is an important way to reduce NO_x emission [17]. At present, major diluents used to lower flame temperature are H_2O, CO_2 and N_2 [18–20]. N_2 could be derived from air separator while high pressure steam could be from heat recovery boiler in IGCC. Though purely adding CO_2 to syngas will increase CO_2 emission, MILD combustion technology, which mixes recirculating flue gas with reactors from inlet of combustor, is a useful way to reduce NO_x emission [21]. So it's necessary to research ignition process of syngas under CO_2-diluted conditions. Das and Sung's [22] research results indicated that when volumetric calorific value of syngas remained the same, 5% and 10% H_2O could increase reactivity and promote autoignition at $p = 3$ MPa. Mathieu *et al.* [23] pointed out that CO_2 addition had negligible effects on autoignition of syngas under low CO_2 content (0.15%). Vasu *et al.* [24] researched autoignition of syngas under high CO_2 content, but they didn't compare their results with conditions without CO_2 dilution. Replacing Ar by N_2 could promote reactivity for $H_2/O_2/N_2/Ar$ mixtures [25], however, to the authors' knowledge, there have no research and reports for syngas mixtures.

Based on published experimental data and reaction mechanisms, the aim of this paper is to research effects of H_2O, CO_2 and N_2 as diluents on autoignition of syngas at gas turbine conditions. Firstly, this paper used three reaction mechanisms above to calculate ignition delay time of syngas and compared them with published experimental data to select the

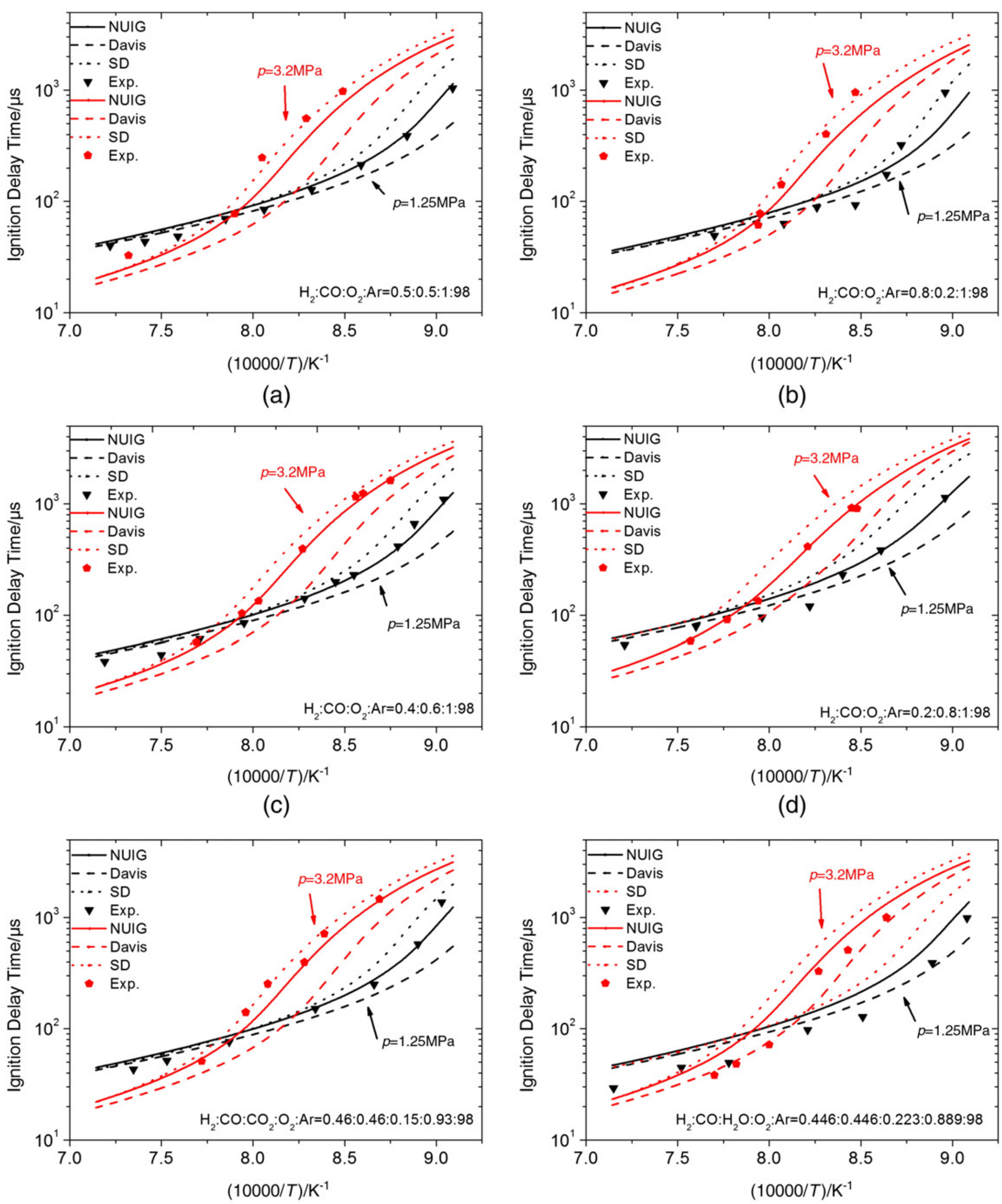

Fig. 1. Comparison with ignition delay of syngas mixtures from experiments [23,29] and calculating results from three mechanisms at $p = 1.25$ and 3.2 MPa, syngas mixtures ($\varphi = 0.5$ and O_2 was oxidizer) were diluted in 98% Ar.