



## Full Length Article

# A shock tube study of ignition delay times in diluted methane, ethylene, propene and their blends at elevated pressures

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## ABSTRACT

Ignition delay times (IDT) of small hydrocarbons at elevated pressures provide a valuable constraint for the refinement of the core small-hydrocarbon sub-mechanisms used in all combustion kinetics. Current knowledge of these core mechanisms is based largely on low-pressure data, with only limited high-pressure data available. To remedy this, the present study focuses on ignition delay times in methane, ethylene, propene and their blends at elevated pressures. IDT measurements were performed in 4% O<sub>2</sub>, balance Ar mixtures, over the temperature range of 950–1800 K, at pressures of 14–60 atm and equivalence ratios of 1 and 2. IDT was determined from recorded sidewall pressure, OH\* emission measurements and fuel time-histories measured using laser absorption at 3.39 μm. These measurements extend the test conditions of earlier studies, with the advantage that they have all been performed at similar conditions and with the same facility and should provide a uniform set of kinetics targets for the evaluation of core small-hydrocarbon mechanisms. This dataset also allowed the temperature variation of the pressure and equivalence ratio scaling for methane and ethylene IDT to be investigated.

## 1. Introduction

There is increasing interest in refining detailed kinetics mechanisms for combustion at elevated pressures. This interest extends to both distillate fuels [1,2] and simpler hydrocarbons, such as methane, ethylene, and propene [3]. Efforts to simplify the detailed mechanisms for distillate fuels have led to the HyChem model that describe the ignition processes of these fuels in two stages: pyrolysis and oxidation [4,5]. In the pyrolysis stage of the model, the large hydrocarbon components of distillation fuels are cracked into smaller hydrocarbons [6], which are subsequently oxidized in the second stage. Because of this change in molecular structure, these models rely on accurate descriptions of the ignition of smaller hydrocarbons such as methane, ethylene, propene and their blends. That is, the models require precise core small-hydrocarbon sub-mechanisms. To refine and validate these core sub-mechanisms, however, accurate ignition delay time (IDT) data are needed for methane, ethylene, propene and their blends, particularly at high pressures where current data are limited. Accurate IDT predictions of methane and alkenes have also become a critical issue in the numerical studies of reacting flows. For example, Wang et al. [7] conducted a systematic high-resolution numerical study of deflagration-to-detonation (DDT) of methane/air mixtures in a detonation tube; Shao et al. [8] studied methane addition effects in a small spark ignition engine; and Pellett et al. [9,10] proposed a simple two-component

surrogate (36% methane/64% ethylene) to simulate the behavior of partially-cracked JP-7. Because of the continuing need to improve modeling of the combustion of small molecule kinetics, further IDT studies, particularly at elevated pressures, are of value.

A significant amount of literature exists for ignition delay times for methane, ethylene, and propene at low pressures. For methane, earlier measurements were mainly conducted at low pressures of 0.5–15 atm [11–17]. A few studies conducted in the last decade, however, probed higher pressures. Huang et al. [18] conducted a series of shock tube experiments to measure the ignition delay of homogeneous methane/air mixtures at moderate temperatures (1000–1350 K) and elevated pressures (16–40 atm). Petersen et al. [19] measured IDT of methane/O<sub>2</sub>/dilute mixtures at pressures ranging from 35 atm to 260 atm. Petersen et al. also investigated the pressure and equivalence ratio dependencies of methane/O<sub>2</sub>/Ar mixtures at 14–52 atm. For ethylene, previous IDT studies were mostly focused on fuel-lean to stoichiometric mixtures close to ambient pressures [20–33]. More recent investigations [34,35] highlight that the predictive capabilities of existing reaction models of ethylene combustion remain unverified and uncertain for fuel-rich mixtures and at elevated pressures, conditions that are important for soot and PAHs formation. Most recently, Davidson et al. [36] measured the ethylene IDT in diluted 4% O<sub>2</sub>/Ar mixtures from 15 to 35 atm. In this study, we measured methane IDT at 14 and 52 atm, and extended the measurement range of ethylene IDT to 60 atm with an

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emphasis on pressure and equivalence ratio dependencies.

For propene, there are only a limited number of earlier investigations. Burcat et al. [37] and Qin et al. [38] conducted their early investigations at pressures below 7 atm. Recently however, Burke et al. [39] conducted a much more detailed study in six different shock tubes and two rapid compression machines (RCMs) over a wide range of conditions. The combination of shock tube and RCM data greatly expanded the data available for validation of propene oxidation models to higher pressures (2–40 atm) and lower temperatures (750–1750 K). In this study, we include a series of propene IDT measurements at 16 atm to provide an overlapping dataset with those performed for CH<sub>4</sub> and C<sub>2</sub>H<sub>4</sub>.

In this study we have also addressed the need for IDT data for mixture blends, as fuel blends may not follow simple linear mixing correlations due to synergistic interactions between different components. We investigated methane/ethylene and ethylene/propene blends at 16 atm.

Finally, the acquisition of an IDT dataset performed at similar conditions and in the same facility enables a more detailed investigation of the subtle variations in temperature dependences of the pressure and equivalence ratio scaling. Here we have also investigated, within the confines of recent detailed kinetics models, the reactions that control the pressure and equivalence ratio scaling for methane and ethylene IDT.

The compositions and test conditions for the nine test mixtures studied are given in Table 1.

## 2. Experimental method

### 2.1. High-pressure shock tube

All IDT experiments were performed using the Stanford high-purity, high-pressure shock tube (HPST). Helium was used as the driver gas and typical test times with uniform conditions were 2 ms; incident shock attenuation rates were monitored and ranged from 1.0 to 3.0%/m. The test time for the high-pressure shock tube was further extended to 8 ms when needed, by tailoring the driver gas with nitrogen. The stainless steel driven section has an internal diameter of 5 cm and was heated to 90 °C. Diaphragms were made of aluminum of 0.5–3.0 mm thickness (with cross-scribing) to allow measurements over a broad range of pressures (2–60 atm). Before introducing the test gas mixture, ultimate pressures in the driven section of less than 10<sup>-5</sup> Torr and leak and outgassing rates of less than 10<sup>-4</sup> Torr/min were regularly achieved. The dP<sub>5</sub>\*/dt (where dP<sub>5</sub>\* = dP<sub>5</sub>/P<sub>5</sub>) values were controlled, and limited to a maximum value of 0.02/ms, by using a driver insert [40]; the effect of this residual dP<sub>5</sub>\*/dt on simulations of the current data was effectively negligible.

Research grade test gases, methane, ethylene, propene, and oxidizer (4% O<sub>2</sub>/Ar) were provided by Praxair. When producing test gas mixtures, the fuel was first introduced into a heated 12.8-liter stainless-steel mixing tank at 110 °C. A test gas mixture of fuel/4% O<sub>2</sub>/Ar was then prepared manometrically and was stirred using a magnetically

**Table 1**  
Gas mixture compositions in mole fraction.

Mixture #	Components	% CH <sub>4</sub>	% C <sub>2</sub> H <sub>4</sub>	% C <sub>3</sub> H <sub>6</sub>	% O <sub>2</sub>	Phi	P (atm)	T (K)
1	CH <sub>4</sub> /O <sub>2</sub> /Ar	1.96	0	0	3.92	1	14/52	1420–1752
2	CH <sub>4</sub> /O <sub>2</sub> /Ar	3.85	0	0	3.85	2	14	1464–1782
3	C <sub>2</sub> H <sub>4</sub> /O <sub>2</sub> /Ar	0	1.32	0	3.95	1	16/60	1095–1317
4	C <sub>2</sub> H <sub>4</sub> /O <sub>2</sub> /Ar	0	2.66	0	3.95	2	16	1122–1268
5	C <sub>3</sub> H <sub>6</sub> /O <sub>2</sub> /Ar	0	0	0.88	3.96	1	16	1255–1488
6	CH <sub>4</sub> /C <sub>2</sub> H <sub>4</sub> /O <sub>2</sub> /Ar	0.54	0.96	0	3.94	1	16	1133–1340
7	C <sub>2</sub> H <sub>4</sub> /C <sub>3</sub> H <sub>6</sub> /O <sub>2</sub> /Ar	0	0.24	0.72	3.96	1	15	1324
8	C <sub>2</sub> H <sub>4</sub> /C <sub>3</sub> H <sub>6</sub> /O <sub>2</sub> /Ar	0	0.53	0.53	3.96	1	15	1211–1329
9	C <sub>2</sub> H <sub>4</sub> /C <sub>3</sub> H <sub>6</sub> /O <sub>2</sub> /Ar	0	0.88	0.29	3.95	1	15	1206–1326

driven vane assembly for 15 min prior to the experiments.

### 2.2. Shock tube diagnostics

Three diagnostics were employed: laser absorption at 3.39 μm, excited OH radical (OH\*) emission near 306 nm, and sidewall pressure. This experiment setup gives detailed information of the reaction progress, and under these operating conditions the ignition delay times defined by the three signals are self-consistent. The differences between the three signals is typically within ± 3% at most operating conditions, but can increase to ± 15% for IDT values below 100 μs. Fuel concentration was monitored using an IR HeNe laser passing through focusing optics, filters, and sapphire windows and with common-mode rejection using reference and transmission LN<sub>2</sub>-cooled InSb detectors. The emission near 306 nm from the A<sup>2</sup>Σ<sup>+</sup> – X<sup>2</sup>Π ((0,0) band) of OH\* was detected using a modified PDA36A Si detector, and a Schott UG5 filter with an optical setup that provided a temporal resolution of 7 μs. Pressure time-histories in the test section were monitored using a Kistler™ piezoelectric pressure transducer model 603B1. The measurement location of all diagnostics was 1.1 cm away from the end wall.

Representative data traces for an example ignition experiment are shown in Fig. 1. These data include pressure traces for the reactive (fuel/oxidizer) and non-reactive cases together with OH\* emission records and 3.39 μm laser absorption measurements. Note that the early time rise of the 3.39 μm signal from 0 to 40 μs is an absorbance artifact related to the convolution of the spatial variation of laser beam and the transition of the reflected shock past the observation port. In this study, IDT was defined as the time interval between the arrival of the reflected shock and the onset of ignition determined by extrapolating the maximum slope of signals back to the baseline. In all cases, this approach provided consistent IDT among the three records. For consistency, all ignition delay data discussed in the following sections use the OH\* emission definition unless stated otherwise. The uncertainty in ignition delay data is typically ± 10% at high temperatures, increasing slightly (to ± 15%) for IDT values below 100 s. this uncertainty is estimated by the theory of propagation of uncertainty with the primary contribution from the ± 1% uncertainty in the initial reflected-shock temperature. One of the main concerns in the acquisition of small hydrocarbon IDT data is the influence of impurities. To minimize the impact of impurities on the IDT measurements, a three-step cleaning procedure was used: physical cleaning with acetone, chemical cleaning with tertbutylhydroperoxide (30% TBHP in H<sub>2</sub>O), and pure oxygen shock cleaning (with T<sub>5</sub> = 2000–4000 K). Following this procedure, highly repeatable IDT data was generated. General estimates of the impurity levels found in Stanford shock tube experiments can be found in Urzay et al. [41].

## 3. Results and discussion

IDT test conditions and values for all experiments are given in the Appendix A. Simulations of the CH<sub>4</sub> IDT measurements were calculated using the FFCM-1 [3] and the ARAMCO Ver. 1.3 mechanisms [42]. Simulation for the neat alkene IDT measurements were calculated using

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