

# Effect of Temperature, Pressure and Equivalence Ratio on Ignition Delay in Ignition Quality Tester (IQT): Diesel, *n*-Heptane, and *iso*-Octane Fuels under Low Temperature Conditions

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## ABSTRACT

Effects of temperature, pressure and global equivalence ratio on total ignition delay time in a constant volume spray combustion chamber were investigated for diesel fuel along with the primary reference fuels (PRFs) of *n*-heptane and *iso*-octane in relatively low temperature conditions to simulate unsteady spray ignition behavior.

A KAUST Research ignition quality tester (KR-IQT) was utilized, which has a feature of varying temperature, pressure and equivalence ratio using a variable displacement fuel pump. A gradient method was adopted in determining the start of ignition in order to compensate pressure increase induced by low temperature heat release. Comparison of this method with other existing methods was discussed. Ignition delay times were measured at various equivalence ratios (0.5-1.7) with the temperatures of initial charge air in the range from 698 to 860 K and the pressures in the range of 1.5 to 2.1 MPa, pertinent to low temperature combustion (LTC) conditions. An attempt to scale the effect of pressure on total ignition delay was undertaken and the equivalence ratio exponent and activation energy in the Arrhenius expression of total ignition delay were determined.

Ignition delay results indicated that there were strong correlations of pressure, temperature, and equivalence ratio under most conditions studied except at relatively low pressures. Diesel (DCN 52.5) and *n*-heptane (DCN 54) fuels exhibited reasonably similar ignition delay characteristics, while *iso*-octane showed a distinct behavior under low temperature regime having a two-stage ignition, which substantiate the adoption of the gradient method in determining ignition delay.

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## INTRODUCTION

An autoignition behavior, characterized by ignition delay time, is an operation limiting factor in diesel engines. Cetane number (CN) has been adopted as an engineering index in representing the autoignition quality of diesel fuel, which typically has the value in the range of 40-55. It is reasonably inversely proportional to fuel's ignition delay such that higher cetane number fuel has shorter ignition delay time than lower cetane number fuel. The minimum cetane numbers set in Europe [1] and North America [2] have been raised recently, even though this does not necessarily translate into higher efficiency. One of reasons is the trend of modern diesel engines toward higher efficiency, and higher speed with direct injection, downsizing and turbocharging. Fuels with higher cetane number have shorter ignition delays, providing more time for fuel combustion. Hence, high speed diesel engines could be operated more effectively with higher cetane number fuels.

The cetane number is measured for a specified fuel in a CFR engine using the standard ASTM D 613 test method [3] by comparing its ignition characteristics with the blends of reference fuels of cetane (*n*-hexadecane, CN = 100) and heptamethylnonane (CN = 15), a highly branched paraffin, or  $\alpha$ -methyl-naphthalene (CN = 0).

An alternative method of measuring autoignition quality related to CN for diesel fuel is by utilizing an ignition quality tester (IQT), which could provide a simpler and robust approach with high repeatability and reproducibility [4], resulting in the derived cetane number (DCN) [5, 6, 7]. The IQT utilizes a constant volume combustion chamber with direct fuel injection into heated, compressed air to simulate unsteady spray autoignition behavior in a diesel engine, where an ignition delay is measured in accordance with ASTM 6890 [8].

Since fuel and air are not homogeneously premixed in an IQT, the measured ignition delay contains both physical and chemical delays, where a chemical ignition delay is typically measured in homogeneous premixed systems, such as shock tubes (ST) [9] and rapid compression machines (RCM) [10, 11, 12, 13, 14]. Note that the autoignition quality of diesel fuel has a good correlation among various empirical measures of auto-ignition propensity, such as the derived cetane number or the total ignition delay in IQT [15].

Recently, operation regimes of diesel engines have been extended to partially premixed, or even near homogeneous fuel/air mixture conditions, especially under low temperature combustion (LTC) environment such as premixed charge compression ignition (PCCI) or homogeneous charge compression ignition (HCCI) mode. Therefore, a single quantity measured at one experimental condition such as the determination of cetane number may not be sufficient in describing autoignition behavior of practical diesel fuels. Moreover, conditions such as pressure, temperature and mixture strength under which autoignition occurs are widely varied in such LTC engines. There are, however, limited data on ignition delay for diesel fuels over practical wide ranges of temperature, pressure and mixture strength. Since IQT could provide well-controlled test conditions, once the operability of IQT can be extended, it may be used as a development and validation platform for kinetics models of novel fuels, especially for LTC mode with very long ignition delay. Several efforts have been made to investigate effects of temperature and pressure on autoignition in a realistic unsteady environment but available data are limited [16, 17]. Additional research is needed towards the temperature and pressure dependences and the influence of equivalence ratio (or mass of fuel injected) on ignition delay.

In a recent work of Bogin et al. [18] wherein a parametric (temperature, pressure and oxygen concentration) study of *n*-heptane, *n*-decane, *n*-dodecane and *n*-hexadecane are described, a wide ranging temperature sweep experiments has been proposed and conducted in the IQT. While their work included experiments performed at constant equivalence ratios to measure the effect of constant fuel mass versus constant equivalence ratio fueling, the most of data presented there were obtained with the mass of fuel injected held constant. It is mainly due to the difficulties changing mass of fuel injected during temperature sweep experiments to held equivalence ratio constant.

In order to enable to maintain a constant global equivalence ratio corresponding to the change of charge air mass (depending on charge pressure and temperature) during temperature sweep experiments in IQT, the mass of fuel injected should be able to be changed within a very limited time between charging the chamber and injecting the fuel (approximately 10 s). To achieve easy and fast control of injected fuel mass in IQT, a variable displacement fuel pump (VDP) has been adopted in a KAUST Research ignition quality tester (KR-IQT) which has a feature of varying temperature, pressure and equivalence ratio. Temperature sweep experiments at constant equivalence ratios were proposed and conducted a series of ignition delay time measurement in a continuous temperature range. Additionally, a new definition of ignition delay in IQT experiment was suggested for the cases with long ignition delays in relatively low temperature conditions.

With these capabilities of KR-IQT, the effects of pressure, temperature and equivalence ratio on the ignition delay in IQT were investigated with diesel fuel and primary reference fuels (PRFs) of *n*-heptane and *iso*-octane to test the proposed method and the definition of ignition delay. A diesel fuel (US-2D, Coryton Advanced Fuels Ltd.) and *n*-heptane have reasonably close values of DCN 52 and 54, respectively. While *iso*-octane has much lower DCN, such that it could exhibit a distinct behavior having a two-stage ignition phenomenon, which could be relevant to provide important information for LTC operation. An Arrhenius expression was used with apparent activation energy and related exponents of pressure and global equivalence ratio in order to express global correlations describing the total ignition delay in IQT for variable pressure, temperature and equivalence ratio.

## EXPERIMENTAL SETUP

### Ignition Quality Tester (IQT) Overview

An IQT is a bench-scale device for the standard ASTM D6890 test to measure ignition delay (ID) and derived cetane number (DCN) of diesel-type fuels. A sample fuel is injected into a heated, temperature-controlled constant volume chamber ( $0.213 \pm 0.002$  L) charged with compressed air having an oxygen concentration of  $20.9 \pm 1.0$  volume %, less than 0.003 volume % hydrocarbons, and less than 0.025 volume % water. The fuel injection system employs a single-hole S-type pintle nozzle (ND-DN12SD12) for liquid fuel injection. Fuel is delivered to the injector with a patented mechanical fuel pump driven pneumatically with air at a pressure of  $1.21 \pm 0.03$  MPa, and injected into the combustion chamber with the nozzle opening pressure of  $18.14 \pm 0.54$  MPa. The injection duration is about 2 ms. Each injection produces a single-shot, compression ignition combustion. Based on ASTM D6890, ID is measured using a pressure sensor from the start of fuel injection to appreciable pressure rise and averaged over 32 injections after 15 pre-injections for stabilization. To define a DCN, the initial charge pressure and air temperature are regulated within the range of  $2.137 \pm 0.007$  MPa and  $545 \pm 30^\circ\text{C}$ , respectively. Calibration reference tests are required with *n*-heptane to have the average of three acceptable ID results within  $3.78 \pm 0.01$  ms.

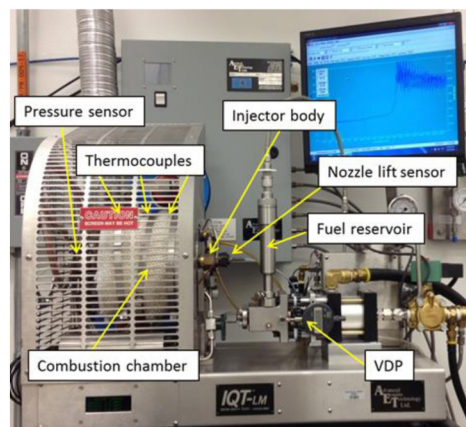


Figure 1. KR-IQT with a variable displacement fuel pump (VDP).

A KAUST Research ignition quality tester (KR-IQT, AET Ltd.), as a photo shown in Figure 1, was developed to measure ignition delays under a broad range of test conditions of charge pressure, temperature and injected fuel mass. Experimental parameters, such as initial charge-air pressure and temperature, chamber surface (skin) temperature, and mass of fuel injected, are well-controlled.

To measure the charge-air pressure and the pressure rise during a combustion event, a pressure transducer (Kistler 601B1) is installed at the end of the combustion chamber. The initial charge air pressure is  $\pm 7$  kPa (1 psi) of the set point. The pressure transducer with an insert is cooled by a coolant jacket to protect the pressure transducer against thermal shock and overheating. The temperature was maintained constant at  $403 \pm 20$  K during the whole test in this study.

The KR-IQT provides three temperature data relevant to charge air temperature; air-front, air-back, and chamber surface temperature, measured by Omega K-type thermocouples at three locations axially along the chamber as shown in Figure 2.

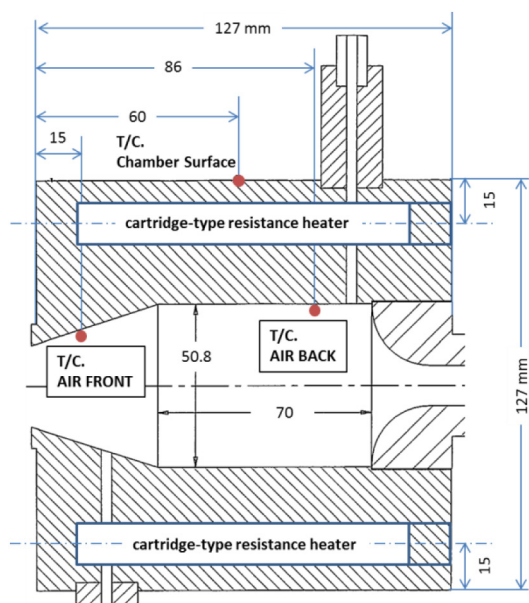


Figure 2. Schematic of KR-IQT combustion chamber with thermocouples.

The inner part of the IQT chamber is heated by nine electrical cartridge-type resistance heaters ( $9 \times 315$  W) embedded in the outer wall of the steel combustion chamber. To avoid heat transfer to the atmosphere, the IQT combustion chamber is well wrapped with an insulating blanket which is made of two parts, a thick (30 mm) inner layer composed of refractory ceramic fibres and a thin outer layer to act as a retainer. The charge-air temperature is fairly uniform in the main portion of the IQT chamber because nine heaters are evenly spaced with circumferential direction and the chamber is well insulated with a thick insulating blanket. As verified by taking several temperature measurements, temperature drops along the length of the chamber exist toward the front of the chamber with a temperature gradient in the axial direction of 0.28 K/mm. The axial temperature drop is due to heat transfer to the coolant flow, which is used to maintain a constant temperature at the injector nozzle ( $323 \pm 4$  K), as specified by the ASTM D6890 standard. A temperature gradient in the radial direction is negligible when the charge-air temperature is

reached steady-state conditions after charging the chamber. The charge-air temperature can be reached steady-state conditions by allowing  $\sim 10$  s to elapse between charging the chamber and injecting the fuel. At constant temperature conditions, the chamber surface temperature was held constant within  $\pm 1$  K of the set point and the charge-air temperatures (air-front, air-back temperature) were repeatable with a range of  $\pm 1.7$  K during 32 injection tests.

While the air-front temperature measured inside combustion chamber proximate to the injector body is used as the test temperature for the ASTM standard, the chamber surface temperature is regarded as the test temperature for this study because this temperature is measured near the center of the chamber and more accurately represents the temperature of the gas throughout the main portion of the chamber. In IQT software, this chamber surface temperature is also used as a set value and appears approximately the average value of the air-front and air-back temperatures. The chamber surface temperature has been used thus far in this study for the Arrhenius type equation and calculation of equivalence ratio and so on.

### Variable Displacement Fuel Pump (VDP)

A conventional IQT experiment is conducted typically under constant injected fuel mass operations. At a constant fuel mass condition, global equivalence ratio ( $\phi$ ) may vary with the changes in the initial charge pressure and air temperature. In this study, IQT experiments were conducted in a wide range of temperature and pressure under constant equivalence ratio conditions by adjusting injected fuel mass conveniently in order to accumulate scientific experimental database. A unique feature of KR-IQT is a variable displacement fuel pump (VDP), which could control injected fuel mass easily by adjusting the displacement of the fuel pump with a system composed of a chain, four stand-offs with turnbuckle-type bolt, and a displacement gauge. The photo of a VDP is shown in Figure 3 comparing with a conventional IQT fuel pump system.

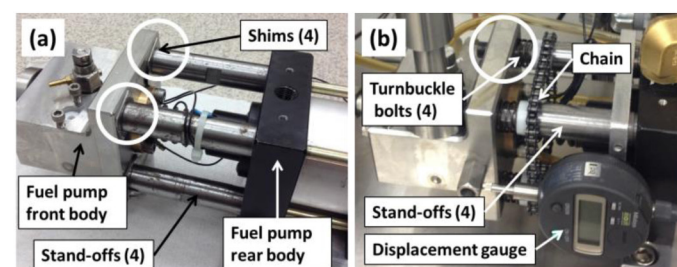


Figure 3. (a) Conventional IQT fuel pump system, (b) a VDP of KR-IQT.

The details of how this VDP actually controls the mass of fuel injected are as follows. In terms of fuel delivery mechanism of an IQT, the delivery volume of fuel specimen from the fuel sample reservoir to the injector nozzle is proportional to the distance between the fuel pump front body and rear body (indicated in Fig. 3a). In a conventional IQT, the amount of fuel injected is controlled by varying the thickness of four (4) shims. In other word, the distance between the fuel pump front body and rear body is adjusted by adding/removing shims. On the other hand, in a VDP of KR-IQT, the displacement between the fuel pump front body and rear body is adjusted by four (4) turnbuckle bolts. A turnbuckle bolt

has right-handed threads on one end and left-handed threads on the other end. The different thread pitches of each end of a turnbuckle bolt result in a high resolution of displacement (0.1524 mm/rev). The rear body of a VDP is fixed on the base plate and the front body is suspended by four stand-offs with turnbuckle-type bolt from the rear body. The four bolts are bound in a chain to make each bolt equally move at the same time. As the bolts turn clockwise, the front body moves backward (i.e. the displacement is decreasing), and vice versa. How accurately this VDP can control the amount of fuel injected is constrained with a resolution of a displacement gauge and depends on fuel properties. For example, with the 0.01 mm resolution of a gauge, the accuracies of fuel amount that this VDP can control were 0.26, 0.27, and 0.34 mg for *n*-heptane, *iso*-octane, and diesel fuel, respectively.

Before ignition tests, mass calibration curves for each fuel are constructed that describes the injected mass as a function of the displacement of a VDP. Several displacements are selected as calibration points, and for each point, twenty (20) consecutive injections are collected in a mass calibration tube. The total mass of the injections is determined by measuring the mass of the container before and after the test which allows direct calculation of the fuel mass per injection. This measuring method is outlined in the operating manual for the IQT in conjunction with the ASTM standard. The steps are repeated until obtaining three consecutive test results which are stable and repeatable with a range of approximately  $\pm 0.3$  mg per injection between test results. The results of the three consecutive stable test results are used to obtain an average weight. The mass calibration curve for test fuels used in this study clearly demonstrate the linear relationship between the displacement of a VDP and the injected mass over the calibrated range of displacement. The linear fits are used to calculate the displacement of VDP required for mass of fuel injected of each test fuel.

### Fuel Specifications and Experimental Conditions

A diesel fuel (US-2D, Coryton Advanced Fuels Ltd.) was chosen to address a need for experimental data showing the effects of pressure, temperature and equivalence ratio on the ignition delay in IQT under low temperature conditions. *n*-Heptane was chosen as a benchmark for comparison, given its much closer DCN value of diesel and well-documented ignition behavior, and for validating the proposed temperature sweep method at constant equivalence ratio with a VDP. While *iso*-octane has much lower DCN, such that it could exhibit a distinct behavior having a two-stage ignition phenomenon, which could be used to validate the definition of ignition delay proposed in this study. The primary reference fuels (PRFs) of *n*-heptane and *iso*-octane were supplied by Sigma-Aldrich and have purities  $\geq 99\%$ . The fuel properties are shown in Table 1. Fuel temperature prior to injection is below initial boiling points of each test fuel by maintaining constant temperatures at the injector nozzle ( $323 \pm 4$  K) and fuel pump ( $308 \pm 3$  K).

Table 1. Fuel physical properties and ignition characterization.

|                               | Diesel      | <i>n</i> -heptane | <i>iso</i> -octane |
|-------------------------------|-------------|-------------------|--------------------|
| initial boiling point (K)     | 458         | 371               | 371                |
| vapor pressure (KPa) at 311 K | -           | 11.07             | 11.7               |
| density (mg/mL) at 298 K      | 855         | 684               | 692                |
| ID (ms) & DCN                 | 3.88 (52.5) | 3.78 (53.8)       | 16.36 (17.8)       |
| (A/F) <sub>stoi</sub>         | 14.6        | 15.08             | 15.03              |

First of all, to clarify the definition of ignition delay time, preliminary tests for *iso*-octane were conducted following ASTM standard method with a constant mass (83.3 mg) of fuel injected in a wide range of test conditions by varying the pressure (2.1, 1.6, and 1.3 MPa) and temperature (720-855 K). Then, experiments utilized a temperature sweep method were conducted in the same range of test conditions mentioned above, while maintaining a constant equivalence ratio of  $\phi = 0.8$  for *n*-heptane. After convincing the temperature sweep method in using the KR-IQT has the validity comparable to the ASTM standard method and it has the advantage of significantly reducing the time required to collect the data, the effects of temperature, pressure, and global equivalence ratio on ignition delay were investigated in a range of temperatures (698-860 K), pressures (1.5-2.1 MPa) and equivalence ratios (0.5-1.7). Experimental test conditions conducted in this study are summarized in Table A in Appendix.

The global equivalence ratio, based on a theoretical stoichiometric air/fuel mixture ratio  $(A/F)_{stoi}$ , was calculated from the mass of fuel injected into the chamber and the mass of air charged inside the chamber. The mass of air was measured by charging the IQT chamber and then exhausting the charge air into a larger gas sampling bag ( $\sim 5$  L) and weighing the total mass of the bag before and after the test on a precise scale. An ideal gas assumption with the chamber surface temperature measured near the center of the chamber was somehow applicable to estimate the mass of air charged inside the chamber, as verified by taking several air-mass measurements at different temperature and pressure conditions. The amount of fuel injected was controlled using the VDP and it was calculated through the mass calibration curve between the displacement of a VDP and the mass of fuel injected. When the mass of air and fuel injected are known, a global equivalence ratio is calculated.

There is a possibility for the exhaust products left over from the previous injection and combustion process. The default exhaust duration in a conventional IQT system was 2 sec. To make sure a complete sweep off exhaust products, the exhaust duration in this study was increased to 4 sec.

## RESULTS AND DISCUSSION

### Definition of Ignition Delay Time

The ignition delay in the present study is defined as the time delay between the start of injection (SoInj) and the start of ignition (SoIgn), based on the simultaneous measurements of the needle lift and the