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Autoignition of pentane isomers in a spark-ignition engine

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Abstract

This paper describes a study on the autoignition of three pentane isomers (*n-*, *neo-* and *iso*-pentane) in a Cooperative Fuel Research (CFR) engine operating at standard, ASTM knocking conditions. The Research Octane Numbers (RONs) of these three fuels are first measured and compared to historical data. Autoignition of pentane/air mixtures in the CFR engine are then simulated using a two-zone model with detailed chemical kinetics. Initial and boundary conditions for these kinetic simulations are systematically calibrated using engine simulation software. Two published, detailed kinetic mechanisms for these fuels are tested with a published NO sub-mechanism incorporated into them. Simulations using both of these mechanisms demonstrate autoignition in the engine for all three pentanes, and that residual NO promotes autoignition, as found in previous studies. Differences between these two mechanisms and the engine experiments are nonetheless observed, and these differences are consistent with those observed in simulations of published rapid compression machine (RCM) data. Comparison of the RCM and the CFR engine modelling also suggests the need for high accuracy experiments and high-fidelity models due to the significant impact that small differences in autoignition timing can potentially produce in real engines.

Keywords: Pentane; Autoignition; Knock; Spark-ignition engine; Nitric oxide

1. Introduction

There are three isomers of pentane: *normal*-pentane, *iso*-pentane (2-methyl-butane), and *neo*-pentane (2,2-dimethyl-propane). Pentanes are significant constituents of gasoline and particularly contribute to gasoline's required vapour pressure. Their content in gasoline typically varies from 10 to 40% by volume worldwide [1,2]. Despite this, the combustion chemistry of pentanes has not been studied as much as that of C1–C4 alkanes or C7–C8 reference fuels. Their chemistry is often embedded in the mechanisms of longer chain alka-

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Table 1
Summary of the standard RON tests of the three pentane isomers (sparking timing = 13°CA BTDC, engine speed = 600 rpm).

	n-Pentane		*neo*-Pentane		*iso*-Pentane	
	This work	API	This work	API	This work	API
RON	61.0 ± 0.1	61.7	88.1 ± 0.1[g]	85.5	91.4 ± 0.1[g], 92.4	92.3
Purity (mol%)	99.3	99.8	99.8	–	99.5	99.8
SKI λ	0.89	–	0.86	–	0.9	–
CCR[a]	5.62	–	6.54	–	6.7[g], 6.86	–
Fuel flow rate (g/s)	0.22	–	0.21	–	0.20[g], –	–
Boiling point (°C)	36.0		9.5		27.7	
Intake air T[b] (°C)	52 ± 1	–	52 ± 1	–	52 ± 1	–
Intake fuel T (°C)	–	–	25	–	45[g], –	–
Intake mixture T (°C)	36	–	59	–	61[g], 36	–

[a] Critical compression ratio (CCR) when maximum knock intensity occurs at mid-scale knock meter reading.
[b] Standard intake fuel temperature compensated for variations in barometric pressure.
[g] Introduced into engine as vapour.

nes without being properly validated, even though experimental data for their oxidation are available from a number of studies [3–7].

This paper therefore examines the autoignition of these three pentanes during a standard, octane rating test in a Cooperative Fuel Research (CFR) engine. Research Octane Numbers (RON) are first measured for the three isomers as it appears that they have only been reported previously by the American Petroleum Institute (API) more than 50 years ago [8], with more recent engine experiments being restricted to motoring studies of *iso*-pentane [9,10]. The autoignition kinetics are then studied at the standard RON test conditions using low order engine modelling, and these results are also compared to modelling of published rapid compression machine (RCM) data.

2. The Research Octane Number (RON)

As properties that characterise the knocking propensity of a fuel in an SI engine, octane numbers are a basic parameter for specifying gasoline. Octane number tests also provide standard, in-cylinder conditions for investigating fuel autoignition, which facilitates potential kinetic investigations that may help understand the chemistry involved in knock and thereby octane rating.

The octane numbers of the pentanes appear to have only been reported by the API in 1940s [8]. Repeating these measurements is considered necessary because the boiling points of these fuels are within the range of ambient temperatures commonly seen in the laboratory (Table 1). In the present study, the RONs of the three pentane isomers are measured using a CFR engine at the University of Melbourne. The engine has recently been used for studying ethanol/gasoline blends [11,12] and liquefied petroleum gases (LPG) [13–15] at ASTM compliant conditions for the research and motor methods [16]. The engine is equipped with a lambda sensor on the exhaust for measuring the air/fuel ratio. Nitric oxide (NO) in the engine exhaust gas is measured using an Autodiagnostics ADS 9000 analyser, which has previously been found to agree closely with the NO analyser in a certification standard, Horiba emission bench.

The RONs measured in the present study are reported in Table 1 together with those from the earlier API study. It is noted that the API study stated that all three pentane isomers were supplied to the engine as a liquid using the standard CFR engine carburettor. This was challenging in the present study for *iso*- and *neo*-pentane, however, since Table 1 shows that these fuels have boiling points that are close to or below typical room temperatures. A gaseous fuel supply was therefore also used for these two isomers using the same setup as in our recent LPG study [13–15].

iso-Pentane, with a boiling point of 27.7 °C, was tested with both vapour and liquid supply. With liquid supply, substantial cycle-to-cycle variations were observed, which is likely due to fuel vaporisation inside the carburettor causing a two-phase flow and 'vapour lock'. The RON measured under this unstable condition was 92.4. This agrees very closely with the API result of 92.3, suggesting that the latter was obtained under similar conditions. Fuelling with *iso*-pentane vapour produced much more stable engine operation, and a RON of 91.4 was measured in this case. The lower RON with vapour fuelling is expected since fuel vaporisation suppresses autoignition by cooling the intake mixture, as is evident by the differing intake mixture temperatures in these cases (Table 1).

neo-Pentane was supplied as a vapour due to its sub-ambient boiling point of 9.5 °C. The fuel line was heated to 25 °C to prevent fuel condensation. The measured RON of 88.1 is higher than the API result of 85.5 where *neo*-pentane was apparently

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