

A CFD Study of Fuel Evaporation and Related Thermo-fluid Dynamics in the Inlet Manifold, Port and Cylinder of the CFR Octane Engine

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ABSTRACT

Knock in Spark Ignited (SI) engines has received significant research attention historically since this phenomenon effectively restricts the compression ratio and hence the thermal efficiency of the engine. The latent heat of vaporization (LHV) of a fuel affects its knock resistance in production engines as well as affecting its Research Octane Number (RON) rating. The reason for this is that evaporative cooling of the fuel lowers in-cylinder gas temperatures resulting in reduced tendency for end-gas auto-ignition. Controlling of the fuel-air mixture temperature to 422 K at the inlet port as per the Motor Octane Number (MON) test method ensures full evaporation of the liquid fuel, and hence LHV is assumed to have little effect during this procedure. LHV therefore has a strong influence on a fuel's Octane Sensitivity (OS) - the difference between its RON and MON values. Since the chemical auto-ignition characteristic of a fuel also strongly influences its octane rating performance, it is of interest to examine the relative effect that LHV has on knock resistance of fuels. LHV is also expected to influence the strength of thermal gradients which develop in the cylinder. These thermal gradients are important, since they have recently been shown to have a strong influence on the rate of pressure rise during end-gas auto-ignition in the Co-operative Fuels Research (CFR) engine used for octane testing. Since the CFR knock meter sensor is triggered by the rate of pressure rise (rather than pressure fluctuation) in a knocking CFR engine, LHV may possess an additional mechanism of influence on the RON rating of a fuel. The current work uses Computational Fluid Dynamics (CFD) engine modelling techniques to provide further insight into the influence of LHV and heat transfer during octane rating by the RON and MON test methods. Fuel LHV and the test engine speeds are shown to influence the in-cylinder temperature gradients at Inlet Valve Closure (IVC). The development of these thermal gradients during compression is shown to be strongly influenced by the combustion chamber wall temperatures and the compression heating behaviour of the fuel-air mixture constituents, in particular the ratio of specific heats, commonly referred to using the symbol γ .

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INTRODUCTION

Octane Number (ON) is a fuel property relating to a fuel's resistance to knock in Spark Ignition (SI) engines. The term "knock" in SI engines is used to describe the engine noise caused by rapid auto-ignition of the unburnt gas. The thermal efficiency of an SI engine is increased by increasing the Compression Ratio (CR). However, increasing the CR increases the unburnt gas pressure and temperature. Since at these higher temperatures, knocking combustion is more likely to occur, the onset of knock in SI engines effectively

limits the CR and thus overall engine efficiency. The design of engines and fuels to reduce knock tendency while allowing higher CR is therefore fundamental to SI engine and fuel development [1], [2].

The presence, or absence, of knock in engines depends primarily on the anti-knock quality of the fuel [1]. The ONs of test fuels are measured based on the octane scale which is defined according to standard octane rating methods for Research Octane Number (RON) [3] and Motor Octane Number (MON) [4]. These tests are performed using the single cylinder Co-operative Fuel Research (CFR) engine.

with engine specifications and operating parameters as given in [Table 1](#) and [Table 2](#) respectively. The ONs of test fuels are measured by comparison at “standard knock intensity” under the same conditions to a mixture of the Primary Reference Fuels (PRFs) *n*-heptane and iso-octane, with iso-octane defined as having an ON of 100 and *n*-heptane an ON of zero. The ON scale is defined by linear volumetric blending of the two, and the ON is given as the % iso-octane in the blend.

Table 1. CFR engine specifications

Stroke	114.3 mm
Bore	82.55 mm
Connecting Rod	254 mm
Compression ratio	variable
Inlet Valve Open	10° ATDC
Inlet Valve Close	34° ABDC
Exhaust Valve Open	40° BBDC
Exhaust Valve Close	15° ATDC
Air-fuel mixture preparation	carburettor

Table 2. CFR engine operating parameters

	RON	MON
Engine speed	600 RPM	900 RPM
Inlet air temperature	325 K	311 K
Inlet mixture temperature	Not specified	422 K

During the MON test, the air-fuel mixture temperature is controlled to 422 K in the inlet manifold to ensure complete evaporation of the liquid fuel before entering the cylinder [5]. The RON test does not require mixture temperature control, and the inlet air temperature is controlled to 325 K upstream of the carburettor. There is thus the possibility of fuel evaporation during intake and compression affecting the in-cylinder temperature and its distribution. The differing operating conditions of the RON and MON tests result in most fuels having different RON and MON ratings. The numerical difference between RON and MON is known as Octane Sensitivity (OS).

Some studies [6], [7] have attributed OS entirely to evaporative cooling effects associated with different classes of fuels. In [8] Swarts and Yates aimed to quantify the in-cylinder fuel evaporation based on the polytropic character of compression. Another study by Wyszynki *et al* [9] investigated the extent of evaporative cooling in the cylinder by comparing volumetric efficiency in port and direct fuel injection engines. Significant improvements in volumetric efficiency were shown to correlate with evaporative cooling potential of fuels tested. Other studies have ascribed OS to a chemical distinction and used detailed chemical kinetics to study the knock phenomenon [10], [10], [11]. Some of this conflict may arise from the challenge in determining the exact value of the gas temperature in the test engine, since conducting temperature measurement in such a highly transient multiphase flow is challenging [10].

This evaporative cooling effect has a further implication when considering knock in the CFR engine. Knock manifests differently in the CFR engine than in conventional production engines, as has been revealed and extensively studied in the work by Yates, Swarts and co-workers in [13], [15] and [16]. During knocking in the CFR engine, the CFR knock meter sensor is triggered by the rate of pressure rise rather than the frequency of knocking pressure fluctuations as is the case for the knock sensor found in production engines. It has been suggested that the thermal gradient set up in the CFR engine due to wall heating and in-cylinder fuel evaporation, could lead to cascading auto-ignition, which in turn could result in the unique pressure development in the knocking CFR engine [16]. This hypothesis was recently supported and further investigated using a multi-zone engine model [16].

For engine knock prediction, it is thus vital to know the magnitude and distribution of the mixture temperature set up during octane rating. The work presented here aimed at providing insight into this parameter and the effect of LHV. Computational Fluid Dynamics (CFD) was used to study the development of in-cylinder conditions. A CFD model of the intake and compression cycle of the CFR engine based on the octane rating tests was developed. The extent of liquid fuel evaporation and the effects of LHV were studied. The two single component fuels iso-octane and toluene were considered and their properties are given in [Table 3](#). Toluene was chosen as a test fuel due to its importance as an aromatic gasoline surrogate blend component and its relatively high LHV. It was thought that toluene's relatively larger evaporative cooling might form part of the explanation for its high OS.

Table 3. Liquid fuel properties, sourced from [18]

	Iso-octane	Toluene
Liquid density [kg.m^{-3}]	688	866
LHV [kJ.kg^{-1}]	270	363
Heat capacity [$\text{J.kg}^{-1}.\text{K}^{-1}$]	2088	1675
Vapour pressure [kPa]	5.5	2.9
Stoichiometric AFR	15.18	13.5
RON	100	111
MON	100	95

ENGINE MODELLING

The overall dynamic characteristics of intake and exhaust flow can be modelled relatively accurately using 1D unsteady fluid dynamic models [18]. In-cylinder processes are generally modelled using 0D thermodynamic models with a two-zone model for the combustion process [1], [20]. In the 0D approach, gas properties and state variables such as pressure, temperature and density represent an average over a zone and hence non-uniformities cannot be accounted for. This approach imposes the assumption that all the air and fuel is fully and uniformly mixed and that liquid fuel either forms part of the wall film or is fully evaporated [7], [22].

Since auto-ignition is a predominantly localized event, spatial variations in flow properties need to be accounted for. Multi-zone models allow either or both the burnt and unburnt zone to be divided into multiple zones, allowing for better spatial resolution of properties. In a recent study by Perumal [16], such a multi-zone approach was implemented together with Flowday's rate-based global auto-ignition model [23]. The difficulty arose in assigning initial properties to each individual zone, since experimental temperature measurement or full 3D simulations would be required. The direct measurement of unburnt gas temperatures still proves difficult, because non-invasive techniques are not very accurate. For example, Coherent anti-Stokes Raman Spectroscopy (CARS) methods can measure in-cylinder temperatures to within 50 K [10], which is still relatively inaccurate compared to the sensitivity of fuel auto-ignition to temperature [24]. The use of 3D CFD for this purpose, notwithstanding its typically limited experimental validation possible, is much less expensive and complex than direct measurements, which hold significant uncertainty in any case. Temporal distributions obtained from CFD can provide estimates of initial and boundary conditions for multi-zone models, and can also be used to optimize the number of zones required for representation of spatial gradients.

COMPUTATIONAL FLUID DYNAMIC AND SPRAY EVAPORATION MODELLING

CFD modelling of fuel sprays in engines is achieved by coupling continuous phase gaseous fluid flow with discrete phase liquid fluid flow. The gaseous fluid flow is governed by the conservation equations for mass, momentum and energy. The conservation of momentum equations are well known as the Navier-Stokes equations. The Finite Volume Method is applied to these equations to solve them in each control volume of the computational domain. The droplets are introduced into the calculated flow field with a certain size, velocity, mass and temperature. The Discrete Phase Model (DPM) solves the trajectory equations, and any other equations describing heat or mass transfer to and from the droplets, by stepwise integration over discrete time steps. Coupling with the continuous phase is achieved via source/sink terms in the Navier-Stokes equations [25], [26]. Spray wall interaction also needs to be considered in the numerical model, since it plays an important part in the mixture preparation. The fuel spray impinges on the manifold walls, the port surfaces and also the intake valve, where it can form a film or splash and subsequently evaporate [26]. Commercial CFD software such as ANSYS FLUENT 12.0 incorporates a wall film model based on the impact energy of the droplet hitting the wall. The magnitude of this impact energy dictates whether a droplet will splash, spread, stick or rebound.

In [27] Chen *et al* combined DPM for tracking of sprays with a 1D gas flow code in order to study the behaviour of

the fuel spray and wall film flow and the effect these have on air-fuel mixing and combustion emissions. The thermal gradients could however not be taken into account in a 1D model. Lui and Karim [28] developed a 3D CFD model, including detailed chemical kinetics, of a Homogeneous Charge Compression Ignition (HCCI) engine to investigate the in-cylinder temperature distribution set up during compression. The engine was based on a modified CFR engine, although liquid fuel was injected directly into the cylinder, allowing for evaporative cooling of the in-cylinder gas. It was found that the combustion chamber wall temperature greatly influenced the auto-ignition timing and its location, and demonstrated the importance of in-cylinder temperature distribution for predicting fuel auto-ignition.

MODEL DEVELOPMENT (METHODOLOGY)

SPRAY EVAPORATION MODEL VALIDATION

Fuel evaporative cooling was investigated by Moran in [6] considering the inlet manifold of the CFR engine. A 1D model was used to model the fuel spray, evaporation and wall film flow. Steady state conditions were assumed, with the model run for representative flow velocities. The computer model simulations were compared to experimentally measured temperatures in a test pipe.

A 2D CFD model based on the work by Moran in [6] and [7] was developed in the present study for validation of the spray evaporation model in ANSYS FLUENT 12.0. The manifold section was modelled using an axisymmetric approach. The cross section modelled had a radius of 16 mm and length of 130 mm. Fuel was injected 30 mm downstream from the inlet, with the pressure outlet 130 mm downstream from the inlet. Air entered the manifold at 5 m.s^{-1} , 325 K and 101.3 kPa. A constant heat flux of 100 W.m^{-1} was applied to the manifold walls. A compression ratio of 7 was used. The fuel droplets were injected with initial diameters and temperatures of $50 \mu\text{m}$ and 295 K respectively, and with zero initial velocity. The steady state solver was used with first order discretization and the realizable k-epsilon turbulence model.

Figure 1 shows the results for the CFD simulation with strong and weak phase coupling together with the measured and modelled data from [7] for iso-octane fuel. Weakly coupled implies that the flow field is solved, followed by the particle tracks, then again the flow field. Strongly coupled implies that once the flow field is solved, the particle tracks and flow field are solved iteratively until both have converged to a final solution.

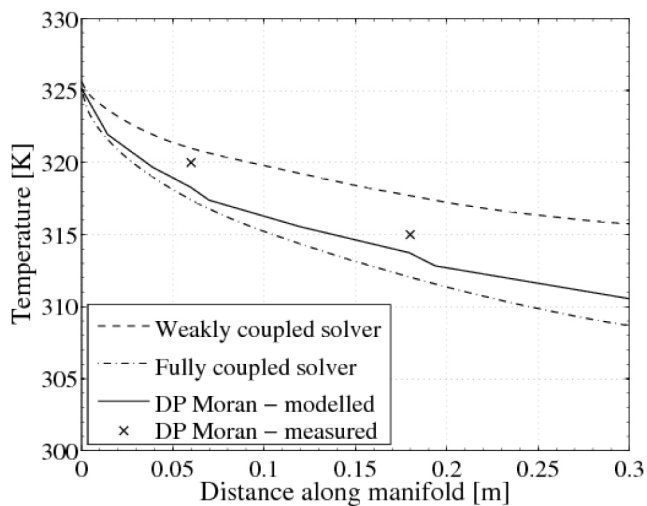


Figure 1. Average static temperature vs. distance along manifold for iso-octane. 0 corresponds to the point of fuel injection.

The modelled and measured data from [7] is seen to be bounded by the data from the weak and strongly coupled simulations. The rate of cooling follows the same trends as that of [7]. The weakly coupled case under predicts and the strongly coupled case over predicts the cooling compared to the measured values. Fortuitously, the unsteady solver - which was used for the full 3D simulations - was a hybrid between the weakly and strongly coupled solver, since coupling between the phases occurred at regular time intervals.

CFR ENGINE CFD MODEL

Geometry and grid

The 3D geometries were created and meshed using ANSYS GAMBIT 2.4. Both the MON (Figure 2) and RON (Figure 3) models consisted of an intake manifold, intake port, inlet valve and combustion chamber. The MON setup consisted of an extra heating manifold section inserted between the intake manifold and intake port. All 3D simulations were run at a CR of 7.8, since this is the CR at which “standard knock intensity” is reached for iso-octane in the CFR engine under RON conditions.

The CFR engine employs a shrouded inlet valve to direct the flow circumferentially along the cylinder walls so as to create swirling flow. The valve shroud geometry was represented as an arc shaped wall which blocked off one half of the valve curtain area.

The bends and protruding structures, such as the heating element and the inlet valve, made structured grid generation in these regions challenging. These regions (manifold and port) were thus meshed with unstructured, tetrahedral elements. Hex-wedge elements were used in all other regions. The in-cylinder grid consisted of a semi-structured mesh with

only hex-wedge elements. The cylinder top and piston face meshes are shown in Figure 4.

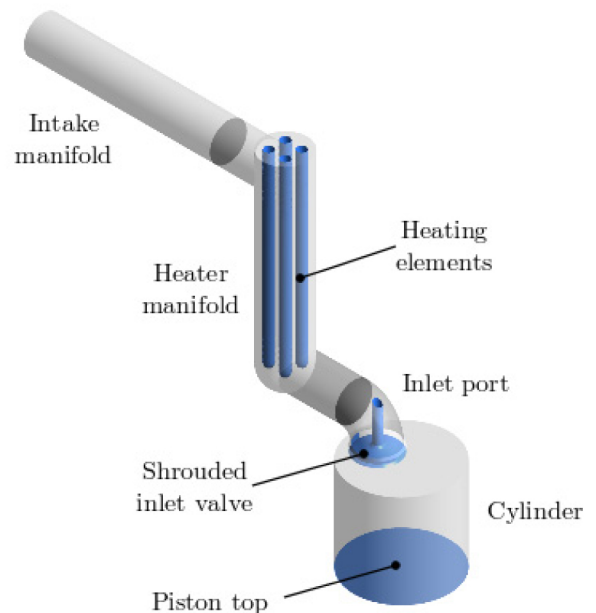


Figure 2. MON model geometry

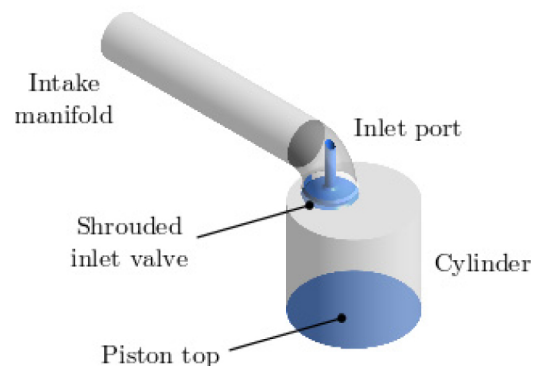


Figure 3. RON model geometry

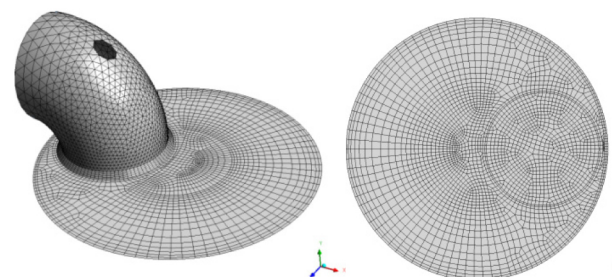


Figure 4. Combustion chamber face meshes. LHS = top. RHS = piston top.

Dynamic mesh layering was implemented with the moving valve and piston boundaries. Mesh layering was applied above and below the inlet valve during valve opening