

An Investigation of Cascading Autoignition and Octane Number using a Multi-zone Model of the CFR Engine

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ABSTRACT

This paper describes a quasi-dimensional multi-zone model of the CFR engine. The engine cylinder was divided into multiple zones containing the unburned air-fuel mixture, which experienced different temperature-pressure histories during the compression stroke and flame propagation phases of the engine cycle. This allowed for the simulation of a temperature gradient within the cylinder, which is postulated to be the cause of the Cascading Autoignition characteristic of the CFR engine.

A Wiebe function description of the flame front propagation was used to describe the normal combustion process; mass and energy were transferred proportionally from the unburned zones to a single burned zone. A Functional Global Autoignition Model (FGAM) was used to describe the autoignition chemistry in each of the unburned zones and an equilibrium approach was used to determine the composition of the burned zone.

This multi-zone model successfully reproduced the non-instantaneous pressure rise seen in knocking CFR pressure traces. A parametric modelling study was then conducted to investigate the influence of inlet pressure, inlet temperature, residual exhaust gas fraction, burn duration, compression ratio and in-cylinder temperature distribution on the cascading autoignition.

Having been calibrated on knocking pressure traces of iso-Octane running under RON 100 test conditions, the model was applied on nine Primary Reference Fuels (PRFs) and a Toluene Standardization Fuel (TSF) under their respective Research Octane Number (RON) test conditions. For each of

the fuels, the calibration constants of the FGAM were optimised to fit a comprehensive set of Constant Volume Autoignition simulations, generated by the CHEMKIN™ Chemical Kinetics Software, based on a well validated Detailed Kinetic Mechanism.

The combination of the computationally inexpensive FGAM that accurately reproduced cool flame heat release with a multi-zone engine model was shown to simulate the post-knock pressure development of a knocking pressure trace in the CFR engine, which the method of using a detailed kinetic model in a simple 2-zone engine model does not. An accurate description of this knock pressure development would enable a more representative simulation of knock intensity as measured in the Octane Rating tests.

INTRODUCTION

Octane rating is the measure of a fuel's resistance to knock in spark-ignition engines. Since knock is potentially very damaging to the engine, it is a key design constraint and operating parameter for engines on the one hand, and production specification for fuel refineries on the other. The ASTM specifications D2699 [1] and D2700 [2], for measuring Research Octane Number (RON) and Motor Octane Number (MON) respectively, make these measurements standard practice for typical gasolines and many gasoline components (the measurement of some alcohol components have proved problematic though [3]).

The operating conditions for the two Octane tests were initially fairly representative of the operating conditions likely to induce knock in early carburetted SI engines. With the advent of Port Fuel Injection, the real life operating conditions gravitated towards those of the RON test.

Kalghatgi [4] proposed an Octane Index measure ($OI = RON - KS$) where K is a constant typical of a given engine and operating condition and S is the sensitivity, $(RON - MON)$. For $0 \leq K \leq 1$, this would result in a linear interpolation between RON and MON. Turbocharged and Direct Injection Spark Injection (DISI) engines (with higher operating pressures and lower temperatures) experience knock outside of the original RON/MON operating envelope [5]. Thus, as is more often the case, $K < 0$ for modern engines. This would require an extrapolation beyond the description space of RON and MON. In order to ensure that this extrapolation is indeed valid, it is extremely important to understand the underlying cause of fuel sensitivity. It was in search of this understanding that this study returned to the ON measuring process in order to understand what is actually being measured.

As a first step in this process, this work was concerned with replicating the unique pressure development seen in knocking CFR engine pressure traces, by using a multi-zone engine model that incorporated the recently developed Functional Global Autoignition Model (FGAM) [6]. This would allow for a better modelled description of Standard Knock Intensity (SKI), which is the metric used to assign Octane Number.

This paper begins with a description of the measurement of Octane number (ON) in the CFR engine and the unique way in which knock manifests under these conditions. The requirements of a model that would be able to describe this behaviour are then discussed with specific emphasis on the choice of the FGAM as the autoignition submodel. The implementation of the multi-zone model itself is then described with discussion of the various simplifications and assumptions made, as well as the calibration of the model to produce the desired pressure development behaviour. Then the results of a parametric study are presented, followed by the application of the model to simulate the RON test for various fuel blends. Finally the strengths and shortcomings of this modelling approach are discussed with a view to incorporating more accurate submodels and input parameters to produce a model capable of ON prediction.

MEASUREMENT OF OCTANE NUMBER

RON and MON both measure fuel knock resistance in the standard single cylinder, adjustable compression ratio, CFR engine under prescribed operating conditions. The CFR engine has a number of design features that make it slightly different to modern production engines. The first is a shrouded inlet valve. This shroud covers half the open valve area and directs flow away from the spark plug and around the cylinder, imparting a high degree of swirl on the in-cylinder flow [7]. The other noteworthy feature is a side-mounted sparkplug, which together with the slow engine speed and heated inlet, create conditions that are more likely

to induce knock at lower compression ratios than standard production engines.

A series of papers by Swarts, Yates and co-workers [8, 9, 10, 11] explored the RON and MON tests in detail by analysing pressure traces of the CFR run under knocking and non-knocking test conditions. Two specific outcomes were important to take note of. The first was that knock manifests differently in the CFR than in standard production engines. In production engines, knock typically involves autoignition of about 5% of the endgas and this is followed by a near instantaneous pressure spike and pressure oscillations audible as the knock sound [13]. In the CFR engine, knock can involve between 30% and 70% of the endgas [9]. A distinct knock-point was observable as shown in Figure 1. This was the point at which the pressure rise rate increased significantly but not in the same instantaneous fashion as the shock wave caused by knock in conventional SI engines. This indicated an accelerated but still non-instantaneous heat release.

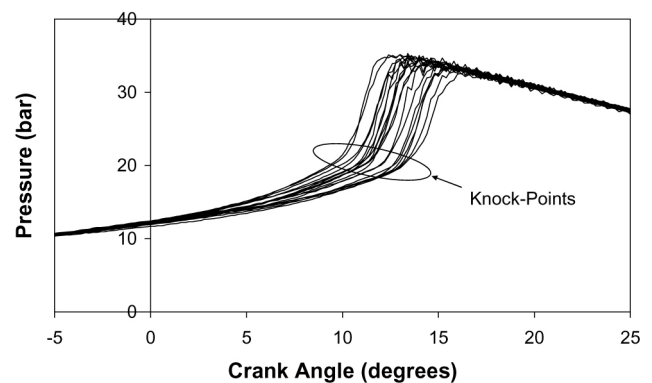


Figure 1. Several Pressure Traces showing the knock-points for PRF80 at SKI under RON conditions

The second important observation concerned the measurement of knock intensity by the knockmeter during Octane rating and specifically Standard Knock Intensity (SKI) [11]. The filtered rate of change of pressure signal is adjusted in magnitude and sensitivity by the METER and SPREAD dials on the knockmeter respectively, before being displayed as a knock intensity reading. This knockmeter reading was less affected by the high frequency pressure oscillations (as would be the case for knock sensors on modern engines [14]) but rather by the unique post knock-point pressure development. In order to model the MON and RON tests for the purpose of predicting octane number, this accelerated pressure development must also be simulated so that a better defined measure of actual SKI can be obtained.

Many current modelling approaches [15,16] used a detailed kinetic autoignition model in a single unburned zone to predict autoignition and then used a measure, such as 30% of unburned mass involved in autoignition, as a proxy for SKI.

Experimental work showed that mass fraction burned at the knock point varied significantly with ON. A graph of the mass fraction burned at knock-point for PRF blends under their respective RON test conditions is reproduced in [Figure 2](#) [10]. It can be seen that as much as 70% of the unburned gas was involved in autoignition for a PRF40 at SKI. Thus using a fixed value of MFB as a proxy for SKI would not be sound assumption. Furthermore these single zone models produced a near-instantaneous pressure rise rate at the knock point [15], which is not consistent with actual knocking CFR pressure traces and so could not be used to simulate readings of knock intensity.

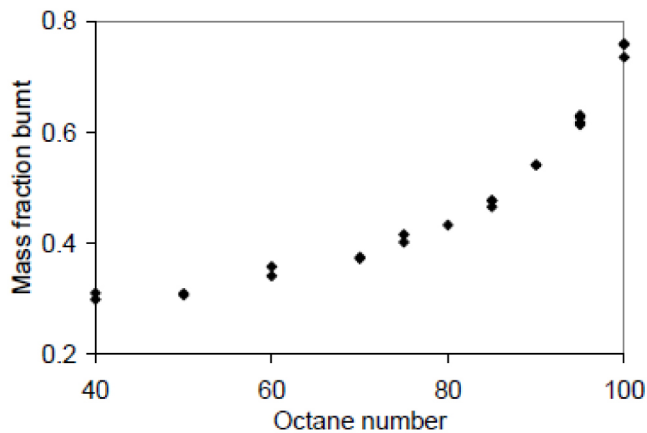


Figure 2. Mass Fraction Burned at Knock Point for PRF40 to PRF100 under RON test conditions [10]

CASCADING AUTOIGNITION

The unique pressure development in the knocking CFR engine had already been noted by Arrigoni et al. [17] in 1974 but surprisingly little work has been done since in attempting to model or explain it. Swarts et al. [18] proposed that it is due to a “cascading autoignition” similar to that seen in HCCI engines. This could be caused by a thermal gradient set up in the CFR engine by wall heating and in-cylinder fuel evaporation, and maintained by the slow engine speed and high swirl generated by the shrouded inlet valve.

A cascading autoignition event is defined as follows: A small portion of the endgas autoignites. The sudden increase in temperature and pressure compresses the adjacent end-gas, which was at a slightly lower temperature, and causes it to also autoignite. This in turn exerts a knock-on effect and autoignition cascades through the endgas faster than the propagating flame speed but still at subsonic velocities.

It is well acknowledged in the literature that knock in SI engines begins with the autoignition of kernels at thermal inhomogeneities [19,20]. However, due to the small mass fraction involved in the knock event and the smaller temperature gradient in the endgas, the pressure rise rate in a

production engine due to knock is near instantaneous and does not show evidence of a cascading autoignition [21]. This partly explains why knock in standard production engines can be so damaging yet is tolerated as standard operating condition in the CFR engine.

In [18] a modelling approach was suggested using multiple unburned zones, each with a different severity of heat loss, to set up the required temperature gradient. It is also suggested that a cascading autoignition beginning near the walls and propagating towards the centre of the cylinder would produce the required pressure development. During the inlet process, the cylinder walls are hotter than the inlet gas and so heating of the gas near the walls could potentially set up such a gradient. It was the aim of the current work to use a similar modelling approach to reproduce the cascading autoignition phenomenon.

AUTOIGNITION MODELLING

The prediction of knock requires a model for the prediction of autoignition of the endgas. Detailed Chemical Kinetic Mechanisms (DKMs), involving thousands of reactions and species, are generally regarded as the most reliable and accurate autoignition models [22] and are commonly used in CFR engine models of the Octane tests such as [15,23]. They are however extremely computationally expensive, even when used in a single unburned zone. Considering the total number of simulations required for this study, the run time associated with such computational expense would not have been feasible.

Reduced or Lumped Mechanisms reduce the number of reactions and species in the system and can potentially provide a good fit of the overall ignition delay over a wide temperature and pressure domain [24]. Mechanisms reduced enough to be computationally efficient were however usually poor at predicting rates of heat release during autoignition, especially the cool flame heat release of “2-stage ignition” fuels [25].

Empirical models based on the Conservation of Autoignition Delay Integral are also currently used to predict autoignition. However even such models that took into account aspects such as cool flame timing and temperature rise [26] did not include predictions of heat release rates and so were unsuitable for the purpose of modelling the pressure rise rate of cascading autoignition

A reaction rate based Function Global Autoignition Model (FGAM) consisting of 9 reactions and 9 species has recently been developed with the specific aim of accurately capturing the heat release characteristics of a wide range of hydrocarbon fuels over varying operating conditions of temperature, pressure, air fuel ratios ($\phi \leq 1$) and residual exhaust gas fraction. This model was able to achieve this by

allowing the coefficients that determine the reaction rates in the mechanism to be adjusted, for a given fuel, to match the autoignition characteristics of either detailed chemical kinetics simulations of that fuel or experimental data.

Since it has been proposed that the sensitivity of fuels can largely be attributed to the difference between single-stage and 2-stage autoignition behaviour [11,27], it was considered important to consider the heat release rates of these processes. The FGAM was used so that the complicated 2-stage autoignition heat release behaviour could be reproduced in a computationally efficient manner. The knock modelling study of [15] specifically did not consider the use of a multi-zone model to describe uneven temperature distribution because of the computational expense associated with their DKM. The use of the FGAM did allow for a multi-zone approach. Additionally the FGAM can potentially be fitted to real, full boiling range gasoline fuels, which is not yet possible with DKMs. The reaction mechanism of the FGAM is summarised in [Appendix A](#) and is more thoroughly described in [28].

The FGAM was fitted to the autoignition profile of a range of PRF Blends and a Toluene Standardization Fuel (TSF). These profiles were generated by the Lawrence Livermore National Laboratory (LLNL) developed detailed chemical kinetics autoignition mechanism described in [29], and run in CHEMKIN™ [18]. For each fuel, 100 constant volume simulations were performed at stoichiometric air-fuel ratio and 15% residual exhaust gas (REG) fraction, spanning initial pressures of 10 bar to 40 bar and initial temperatures of 600 K to 1200 K. The parameters of the FGAM were then optimized by a Particle Swarm Optimisation Method [30] to best match the temperature-time traces of the corresponding CHEMKIN runs.

An example of the overall autoignition delay fit for a PRF80 blend is shown in [Figure 3](#). The average error in the overall ignition delay for this fit was 9%. The fitness function to be minimised for optimisation was the area between the temperature-time curves of the DKM and FGAM simulations, as per [Eqn 1](#).

$$err = \frac{\int_{t=0}^{ID} |T_{DKM} - T_{FGAM}| dt}{T_{AI} \times ID} \quad (1)$$

Where *err* is the error in fit, *t* is time, *ID* is overall ignition delay, *T_{DKM}* is the temperature predicted by the DKM, *T_{FGAM}* is the temperature predicted by the FGAM and *T_{AI}* is the temperature above which autoignition was assumed to be complete. *T_{AI}* was set to 1500K to provide balance between fitting overall ignition delay and cool flame behaviour.

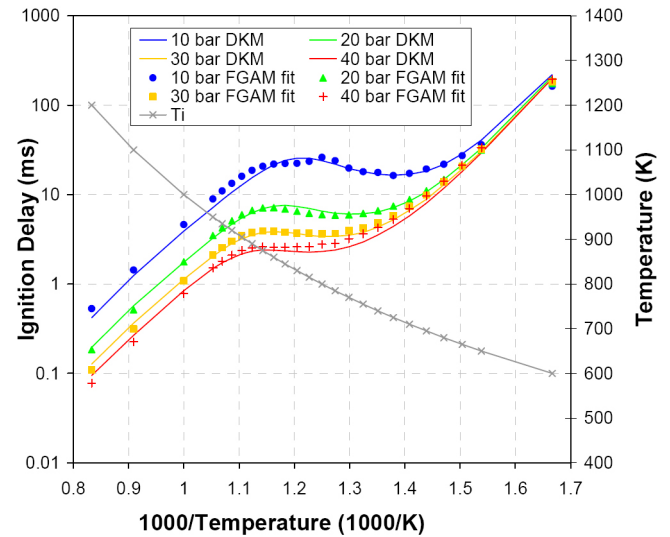


Figure 3. Overall Ignition Delay Fit of the FGAM to DKM simulations for PRF80 blend at $\phi = 1$ and REG = 15%

In this way the overall ignition delay as well as the cool flame heat release could be targeted. [Figure 4](#) shows examples of these temperature-time traces. This fit of the FGAM showed a slight under-prediction of the cool flame ignition delay and ceiling temperature and a slight over-prediction in post-cool flame ignition delay. However the overall trends for these parameters were directionally consistent. Floweday [25] notes that the differences between Detailed Kinetic Models can be as much as 38% in overall ignition delay so an overall fit of less than 10% may be regarded as quite acceptable.

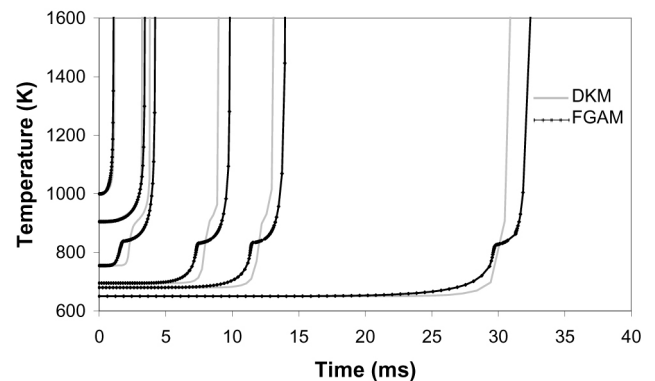


Figure 4. Examples of Temperature vs Time traces for PRF80 at 30bar and various initial temperatures showing FGAM fit to DKM simulations of overall ignition delay and cool flame behaviour

The FGAM calibration coefficients obtained in this study are provided in [Appendix B](#). The average error in fit was between 6% and 12% for PRF blends and 15% for the TSF blend.

MULTI-ZONE ENGINE MODEL

The engine model used in this investigation was a multi-zone quasi-dimensional model that incorporated some of the traits of traditional 2- and 3-zone SI models [16] and thermally stratified multi-zone models used in the study of HCCI engines [31]. The multi-zone model was set up on a simple modular basis with various initial assumptions to show proof of concept in its implementation. The intention of this was to emulate the cascading autoignition seen in the CFR engine through the modelling of a temperature gradient within the engine cylinder.

The unburned gas in the cylinder was divided into multiple zones by volume. The division was done so as to nominally represent an annular distribution of zones within the cylinder (as shown schematically in Figure 5) but the zones themselves were zero-dimensional. The outer most zone represented a thermal boundary layer for purposes of heat transfer to the cylinder walls. The other zones were modelled as adiabatic, with no mass transfer between the unburned zones. These zones could then each be assigned unique initial temperatures to represent an initial thermal gradient at Inlet Valve Closure (IVC). It is proposed that such a thermally stratified annular distribution may be set up by the high degree of swirl in the CFR due to the shrouded inlet valve.

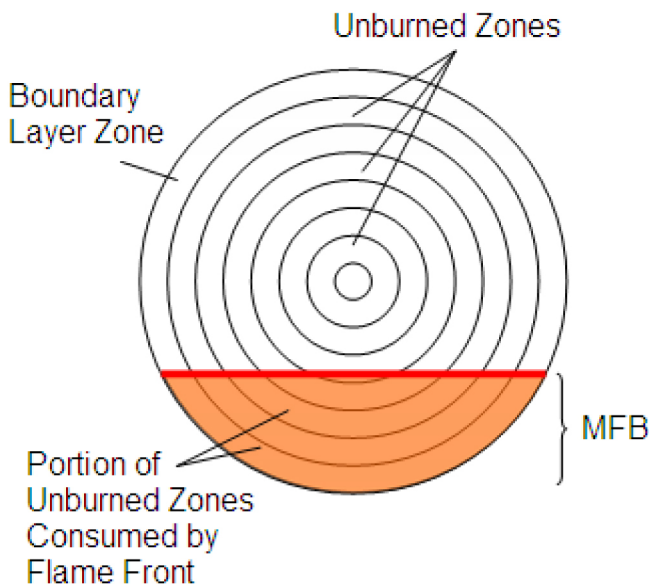


Figure 5. Schematic of concentric Unburned Zone reference layout showing linear consumption by the advancing flame front

The adiabatic zone assumption was adopted to simplify the simulation of the autoignition chemical reactions. Modelling any actual heat transfer that would occur in the turbulent cylinder environment would be extremely challenging in a quasi-dimensional model such as this. It is proposed instead that an adiabatic initial distribution can be found that results

in the same temperature gradient at the point of knock, which would achieve the required result.

IMPLEMENTATION

The engine model was implemented as shown in the flowchart in Figure 6.

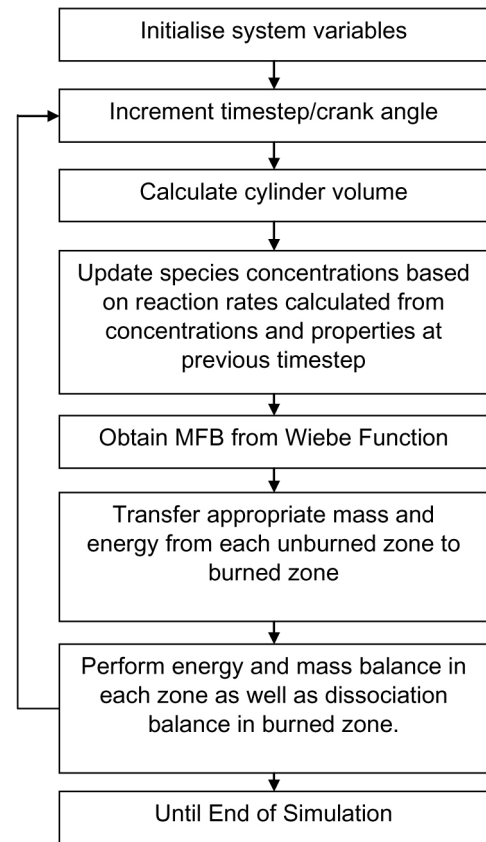


Figure 6. Simulation Algorithm of the Multi-zone CFR engine model

At each timestep the total volume of the cylinder was calculated from the formula [13]

$$\frac{V}{V_c} = 1 + \frac{1}{2}(r_c - 1) \left[R + 1 - \cos \theta - \sqrt{R^2 - \sin^2 \theta} \right] \quad (2)$$

(where V is the instant cylinder volume, V_c is the clearance volume, r_c is the compression ratio, R is the conrod-crank ratio and θ is the current crank angle). For each zone i , an energy balance

$$Q - \left(\frac{p_{i,t} + p_{i,t-1}}{2} \right) (V_{i,t} - V_{i,t-1}) - (m_{i,t} u_{i,t} - m_{i,t-1} u_{i,t-1} + \delta m_{in} u_{in} - \delta m_{out} u_{i,t}) = 0 \quad (3)$$

(where Q is the heat transfer into the zone, p is the pressure, m is the mass, u is the internal energy, and δm is the mass transferred. The subscript i represents the property of that zone, t the current timestep, in transfer into the zone and out transfer out of the zone) and the ideal gas law equation:

$$p_{i,t}V_{i,t} - m_{i,t}R_{i,t}T_{i,t} = 0 \quad (4)$$

(where R is the mixture gas constant) were set up at each timestep t .

The zones were linked by setting the pressure of each zone to be equal to the total cylinder pressure and by the volume balance,

$$V_{cyl} - \sum_{i=1}^{n \text{ zones}} V_i = 0 \quad (5)$$

For n zones then there would be n temperatures, n volumes and the overall cylinder pressure values to solve at each timestep (a total of $2n + 1$ variables). A total of n energy balances, n ideal gas law balances and 1 volume balance also gave $2n + 1$ equations to solve. Such a system of k equations in k unknowns could be solved by a multi-variable Newton's Method [32] by iteratively setting

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \mathbf{J}_n^{-1} \mathbf{f}_n \quad (6)$$

Until $\mathbf{x}$ converged, where $\mathbf{x}$ is the vector of variables, $\mathbf{f}$ is the vector of functions to be set to 0 (ie. the balance equations) and $\mathbf{J}$ is the Jacobian matrix of $\mathbf{f}$.

Flame Propagation Modelling

The flame propagation of normal combustion was modeled by means of a Wiebe function representing the mass fraction burned (MFB), where the values of a , m , θ_{ign} and $\Delta\theta$ burn in [Eqn. \(5\)](#) were tuned to match experimental data.

$$\chi = 1 - e^{-a \left(\frac{\theta - \theta_{ign}}{\Delta\theta_{burn}} \right)^{m+1}} \quad (7)$$

The flame front was regarded as being infinitely thin and consumed mass in the unburned zones in a linear fashion as shown in [Figure 5](#). Note that this does not necessarily mean that the flame itself proceeded linearly. As the flame front expands, it compresses the unburned gas ahead of it. This together with the swirl generated by the shrouded inlet valve would distort any original geometric distribution of the unburned zones. The zone consumption profile of the reference configuration would therefore not be the same as

the geometric flame development profile. With the side mounted spark plug of the CFR, a simple linear consumption profile was used as the best first approximation.

For each MFB value, the segment corresponding to the MFB of the total cylinder volume was calculated and overlaid on the reference zone distribution profile. The appropriate incremental mass and enthalpy from each of the unburned zones lying within the burned segment was then transferred to the burned zone. An enthalpy balance involving the change of species from reactants to products accounted for the heat of combustion.

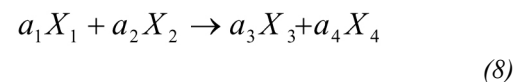
In the burned zone, the Water-Gas Shift and CO_2 dissociation equilibrium reactions were used to determine the final burned temperature by minimizing Gibbs Free Energy and balancing C , H and O atoms. This added 5 additional equations and 5 concentration variables of CO_2 , CO , O_2 , H_2O and H_2 , to the system to be solved in [Eqn. \(6\)](#).

Heat Transfer

Heat Transfer was assumed to occur from the burned zone and the designated boundary layer unburned zone only. A Woschni correlation [13] was used to calculate the convective heat transfer coefficients. The proportional cylinder wall area was apportioned between the burned and unburned zones on a cylinder volume fraction basis. Although the coolant temperature for both RON and MON tests are specified at 100°C , a wall temperature of 150°C was used for these simulations, based on experimental measurements using surface thermocouples in the CFR [33]. Some variation in the Woschni coefficients was experimented with but, since these did not have a significantly large effect on the model results, it was decided to use the original textbook values for this initial study.

Autoignition Chemistry

In each unburned zone the chemical reactions specified by the FGAM were allowed to proceed with reaction rates calculated from the instantaneous temperature, pressure and species concentrations. For a given reaction



The reaction rate (RR) was calculated by

$$RR = [X_1]^{n_1} [X_2]^{n_2} p^{np} A e^{-B/T} \quad (9)$$

(where n_1 , n_2 , np , A and B are reaction rate coefficients) For each species X then, its rate of change of concentration with time was calculated by

$$\frac{d[X]}{dt} = \sum_{i=1}^{n \text{ reactions}} b_i R R_i \quad (10)$$

Where the b_i are the number of moles of X in the reaction equation of reaction i (the corresponding a value in Eqn (8)). Note that if X is a reaction product, $b_i > 0$; if X is a reactant, $b_i < 0$ and if X is not involved in the reaction then $b_i = 0$.

In each zone, a system of ordinary differential equations of species concentration with respect to time was thus defined. The differential equations were then solved within each chemical timestep before the physical balances, described in the sections above, were used to solve for the pressures, volumes etc in the next physical timestep. An energy balance was performed in each unburned zone at the end of each chemical timestep to realize any heat release from the intermediate reactions. To increase the resolution of the chemical timescale, multiple chemical timesteps were taken within each physical timestep based on an adaptive timestep method. Once an unburned zone had reached a critical temperature (in this case set to 1500 K) it was regarded as having autoignited and its contents were set to the same fractions as the burned zone to ensure the correct final equilibrium temperature.

MODEL CALIBRATION

Each engine model simulation was run from Inlet Valve Closure (IVC) to Exhaust Valve Opening (EVO). Determination of IVC cylinder temperature distribution and residual exhaust gas is extremely challenging to determine experimentally [34]. For this preliminary investigation, initial conditions were selected to best match experimental pressure traces and were checked against a basic engine breathing model and values from literature [35] to ensure these conditions were within reason.

A large collection of knocking and non-knocking CFR pressure traces from previous studies [8, 9, 10, 11] was used to calibrate the model and validate its results. These experiments were performed in a CFR engine fitted with a water-cooled piezo-electric pressure transducer with various PRF and TSF fuels under standard RON test conditions. The raw pressure trace and filtered rate of pressure change data was kindly supplied by the authors. The results of these experiments are presented alongside the model results where appropriate and referenced as [12]. Where average values from a series of engine cycles are used, error bars represent 1 standard deviation in distribution of the data.

The model parameters were adjusted to match the experimental runs of PRF100 knocking at SKI under RON100 conditions, and at RON80 test conditions to

compare non-knocking traces. Features of the pressure traces to be matched were: pressure development during compression, pressure development during normal combustion, peak pressure and location of the knock point. A comparison of the non-knocking and knocking RON pressure traces are given in Figures 7 and 8 and a list of the operating parameters used is given in Table 1.

Table 1. Simulation Parameters used in the Multi-zone Model to fit experimental pressure traces

IVC	-146	CAD
EVO	140	CAD
Engine Speed	600	rpm
Bulk Temperature at IVC	400	K
Temperature Gradient at IVC	20	K
Pressure at IVC	0.97	bar
Residual Exhaust Gas Fraction at IVC	20%	
θ_{ign}	-18	CAD
$\Delta\theta_{burn}$	48	CAD
Wiebe a	9	
Wiebe m	5	
Number of Unburned Zones	20	
Number of Timesteps	600	

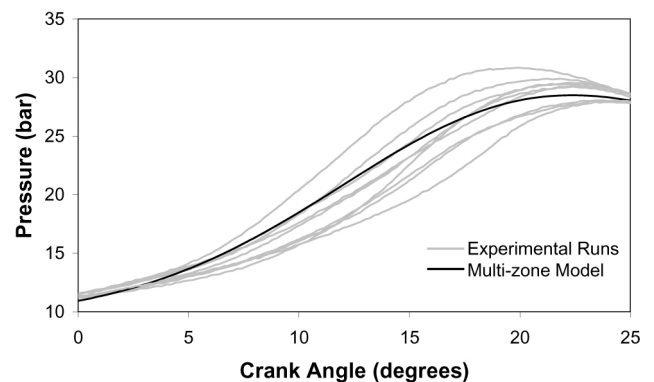


Figure 7. Comparison of the non-knocking pressure trace generated by the Multi-zone CFR Model with PRF100 at RON80 conditions with experimental pressure traces from [12] (burn duration 52 CAD)