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# A Real-Time Capable Mixing Controlled Combustion Model for Highly Diluted Conditions

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## Abstract

A new real-time capable heat release rate model is presented that captures the high dilution effects of exhaust gas recirculation (EGR). The model is a Mixing Controlled Combustion type with enhancements to account for wall impingements, pilot injections, charge dilution caused by EGR at part load. The model was parameterised in two steps using a small set of measured data: the majority of model parameters were identified without EGR before identifying additional EGR related constants. The model performance was assessed based on key metrics: start of combustion; peak heat release and point of peak heat release and cylinder pressure. The model was evaluated over the full engine speed, load and EGR operating envelope and cylinder pressure metrics were predicted with  $R^2$  values above 0.94. With EGR, the model was able to predict qualitatively and quantitatively the performance whilst being parameterised by only by a small dataset. The model can be used to enable the engineering of robust new control algorithms and controller hardware for future engines using offline processes.

**Keywords:** Diesel Combustion, Real Time model, Exhaust Gas Recirculation, Engine Model

## 1. Introduction

Diesel engines are used in a significant proportion of automotive applications due to their inherent high efficiency compared to Gasoline engines. However, Diesel engines suffer from higher emissions of nitrous oxides (NO<sub>x</sub>) and particulate matter due to the nature of the combustion processes. To address this problem, Diesel manufacturers are having to resort to an increasing number of active emissions

1 control technologies such as air management and exhaust gas recirculation (EGR), Lean NOx traps  
2 (LNT) and selective catalytic reduction (SCR) [1]. These systems all require careful design and  
3 management if the high efficiency of the Diesel engine is to be maintained. Virtual development of  
4 the complete system is a promising way of being able to design and optimise the engine system before  
5 development hardware is available. The virtual development can consist of many system models or of  
6 models working in parallel to real hardware, such as hardware-in-the-loop approach (HiL). Accurate  
7 and real-time capable mathematical models are a pre-requisite for this approach [2].

8 Combustion is the key process for any engine as it affects all other engine subsystems. Therefore, real-  
9 time capable combustion models are an essential tool to enable virtual development and HiL  
10 methodology. For example, the real-time model replaces real engine hardware and allows the engine  
11 controller to be trialled can be tested at very early stages of the design process, and much more  
12 intensely than could be achieved though real experiments. The model emulates each of the engine's  
13 sensors and actuators however, the method is underpinned by the accuracy of the mathematical  
14 model and the ability to parameterise the model based in a way that is predicts engine performance  
15 well in extrapolated regions.

16 The recirculation of exhaust gases (EGR) to control NOx emissions in Diesel engines poses specific  
17 challenges through thermal, chemical and dilution effects that need to be accounted for within the  
18 combustion model. EGR critically affects the combustion process by delaying ignition and reducing the  
19 reactivity of the cylinder charge [3]. These effects need to be captured in a model that can easily be  
20 parameterised using only small amounts of experimental data.

21 The aim of this paper is to create a crank angle resolved, real-time capable, Diesel combustion model  
22 that captures the effects of EGR. The empirical model parameters must be generally applicable and  
23 determined using only a small number of engine operating points such that they could be established  
24 from an early prototype build or from a higher order modelling environment [4, 5]. The model must  
25 be able to predict combustion with EGR rates of up to 40-60% (equivalent to up to 5% CO<sub>2</sub> by volume

1 in the cylinder charge). This is relevant for small, high speed Diesel engines in passenger car and light  
2 duty truck applications for the foreseeable future.

## 3 **2. Background**

### 4 **2.1. Reduced order combustion model types**

5 As most combustion, related control strategies could be developed using cycle average quantities such  
6 as the peak heat release, maximum cylinder pressure and IMEP [6], the first reduced order models for  
7 real-time applications were Mean Value Engine Models (MVEM). This approach essentially used look-  
8 up tables for the cycle averaged values as a function of engine operating points (e.g. engine speed,  
9 fuelling quantity, injection timing, EGR rate...) [2, 7-9]. As these models run on a cycle-by-cycle basis,  
10 they can easily be made to run many times faster than real time [10-14]. More recently,  
11 thermodynamic based MVEMs have been proposed based on ideal thermodynamic cycles thus  
12 including a description of the physical processes and reducing the amount of empirical data required  
13 to obtain an accurate model [15]. Whilst these MVEMs do not simulate the full combustion process,  
14 they do allow key quantities such as peak pressure and temperature to be estimated.

15 As the computing power of HiL simulation machines increased, real-time crank-angle resolved models  
16 have been proposed that calculate the evolution of in-cylinder pressure during the engine cycle. This  
17 type of model provides a breakdown of the time related variations in cylinder conditions throughout  
18 the engine cycle. These models have the advantage of being able to estimate the average state of the  
19 charge and have been linked to emissions that capture specific mechanisms of formation of NO<sub>x</sub> [16-  
20 20] and soot [21].

21 These models typically comprise:

- 22 - A combustion model to predict the heat released from combustion.
- 23 - A cylinder model to calculate the gas properties and thermodynamic state of the charge.

1 The crank angle resolved models can be split into 2 categories: “single zone” models or quasi  
2 dimensional models.

3 The term single zone is expressed in italics as it refers to models that consider the heat released from  
4 combustion to influence a homogeneous pressure and temperature throughout the combustion  
5 chamber. The properties of this single zone may be calculated from the different compositions of fresh  
6 air, burnt gas and unburned fuel. One of the major challenges of these single zone models is in defining  
7 a set of model coefficients that are not specific to each operating point of the engine [22].

8 Quasi-dimensional models break down the combustion chamber into small packets and therefore  
9 provide a spatial decomposition of the combustion process [23-25]. Most are built on the work of  
10 Hiroyasu [26, 27]. They are still built on empirical equations and their superiority over simple models  
11 is not yet proven [22]. Recent publications presenting these types of models can run with a calculation  
12 time of less than 1s per engine cycle, but these are still too slow for real time applications [28]. Gao et  
13 al. [29] simplified a quasi-dimensional model [20] to increase the run time. They limited the number  
14 of zones to 2, thus increasing the calculation time by a factor of over 100 to nearly real-time. An  
15 alternative approach was presented by Bittle et al. [30] who used the multizone approach for  
16 calculating local gas compositions whilst maintaining a single zone model for the heat release to  
17 reduce the model calculation time.

## 18 **2.2. Real-time Phenomenological combustion modelling**

19 Crank-angle resolved Combustion models for real time simulation models typically treat the engine  
20 cylinder as a small number of control volumes, composed of gasses of various species representing  
21 the fresh air, unburnt fuel and burnt products. In a single zone more, the combustion chamber is  
22 represented by variable size control volume (Figure 1). The control volume exchanges mass through  
23 the fuel injector, the intake and exhaust valves and via blow-by flows seeping through the piston ring  
24 pack. Energy is exchanged with the control volume through the combustion of fuel, heat transfer to

1 the combustion chamber walls and through work transfer to the piston. Performing an energy balance  
2 on the control volume yields equation 1 [31].

$$dU = dQ_C - dQ_{HT} - dW + dH_{inl} - dH_{exh} - dH_{bb} \quad 1$$

3  
4 This work is focussed exclusively on the calculation of the combustion heat release term ( $dQ_c/dt$ ) for  
5 a Diesel engine with EGR. The combustion models found in the literature typically fall into two  
6 categories:

- 7 - **Shape Functions**: the most common is the Wiebe model [32, 33] although other shape  
8 functions or Neural Networks are also used [9, 34]. These models aim to replicate previously  
9 measured behaviour. Sometimes the model parameters are loosely linked to physical  
10 parameters [35] but empirical correlations are almost always required [36, 37].
- 11 - **Physics Based**: these models are based fuel availability and an assumption of combustion  
12 process and the most common is the mixing controlled combustion (MCC) models. Although  
13 these models comprise of a significant number of empirical constants, the amount of  
14 experimental data required to parameterise these models is substantially less than for shape  
15 functions.

16 The shape functions have achieved a high accuracy in terms of mathematically replicating the  
17 combustion process: they have been shown to predict the angle of 50% burn (CA50) to within +/-1deg  
18 [38] and peak cylinder pressure to within 2-7% [37]. However, to achieve this level of accuracy, a  
19 significant amount of model training data is required [38]. Consequently, they are only useful if  
20 considerable amount of data can be used. The Wiebe combustion models published in the literature  
21 typically require different model parameters for each engine operating point [35, 38, 39] or use  
22 empirical correlations to describe how the parameters vary with operating condition [37, 40, 41].

1 The MCC model was originally proposed by Chmela and Orthaber [42] for large bore engines with the  
2 intention of introducing more physical based equations to reduce the amount of model training  
3 required. These models are based on the turbulent energy resulting from the injection of fuel and is a  
4 reasonable representation of the combustion process during the diffusion phase. However, Dec's  
5 phenomenological model of Diesel combustion defines two phases [43]:

- 6 - a premixed phase resulting from the detonation of fuel that accumulates before combustion  
7 - the base MCC model is weak in this area [44]
- 8 - A stoichiometric diffusive combustion phase where combustion is controlled by the rate of  
9 mixing of fuel with the surroundings – well captured by the MCC model.

10 This means that mixing controlled combustion yields a good estimate of combustion at high loads,  
11 where much of the combustion is diffusive, but is much less accurate at part load conditions where  
12 significant amounts of fuel combustion are in the premixed mode [45-49]. Some empirical adaptations  
13 of the MCC models have been proposed based on fuel preparation [50-53], although these re-  
14 introduce the need for large training data sets. Chmela et al. [45, 47] proposed complementary models  
15 for capturing the premixed combustion on a semi-empirical basis. Katrasnik et al. [19, 53] splits the  
16 combustion into three phases by splitting the diffusion combustion into a rich combustion (in the  
17 centre of the spray) and a lean combustion (edges of the spray). Rezei et al. [54] augmented this mode  
18 with a spray model and included the effects of swirl and squish in the turbulent kinetic energy model.  
19 The accuracy of these models tends to be lower with CA50 errors typically +/-2°CA and IMEP +/-1bar  
20 [54].

21 An alternative MCC model has been proposed by Barba [50]. This model includes the evaporation of  
22 fuel, the flame propagation in the pre-mixed zone and mixing controlled combustion linked to the  
23 characteristic mixing frequency. This model has been the focus of several recent applications where a  
24 single set of parameters has been used across the engine operating map [18, 55, 56]. These models  
25 have accuracies for IMEP of +/-1bar, for CA50 +/-2°CA and for peak cylinder pressure +/-3bar [18, 55].

1 The MCC models have typically been able to be parameterised with fewer test points than the shape  
2 function equivalents [5, 55]. For specific area of the engine operating range they have been  
3 parameterised with a single set of coefficients [44, 45], typically using data from up to 20 engine  
4 operating points [18]. This means they are better suited for use earlier in the process as data for a  
5 small number of operating points can be obtained from higher order simulations [4] or from single  
6 cylinder research engines [55].

### 7 **2.3. Accounting for EGR in combustion models**

8 EGR presents a significant challenge for MCC combustion modelling as the dilution emphasizes pre-  
9 mixed combustion. In displacing the fresh air, EGR will reduce the available oxygen in the cylinder  
10 (dilution effect), increase the thermal capacity of the trapped gases (thermal effect) and increase  
11 dissociations reactions (chemical effect) [57-62]. The net result of EGR on apparent heat release is  
12 illustrated in Figure 2 for a 2.0L Diesel engine operating at a low load. Ignition delay is increased  
13 meaning more fuel will contribute to premixed combustion but the peak heat release is reduced as  
14 the volume of the combustion flame is larger (dilution effect) and the gases in the flame have a high  
15 specific heat (thermal effect).

16 In practice, EGR also affects the engine breathing characteristics because of thermal throttling [61]  
17 and high levels of EGR also cause an increase in cycle-to-cycle and cylinder-to-cylinder variability,  
18 reducing engine stability [63].

19 For shape function heat release models which are calculated at each engine operating point, the  
20 effects of EGR are captured in the individual coefficient that describe any operating point with EGR  
21 [38]. For those models seeking correlations between Wiebe coefficients and operating point, the EGR  
22 rate has been used explicitly [38, 40]. Finesso and Spessa also calibrated their empirical model over  
23 six operating points, but focussed their model only on part of the engine operating envelope [51]. The  
24 combustion delay parameters for pilot and main injections were estimated as empirical functions of



1 charge density, oxygen concentration and fuel injection pressure. This approach has also been  
2 adapted for from phenomenological models [50, 52, 64].

3 Correction factors to the MCC combustion models have also been proposed to account for EGR have  
4 been proposed [46, 48] and implemented in some models. The simplest approach consists of  
5 implementing EGR adjustment factors to the diffusion combustion [46, 48, 65, 66]. Wurzenberger and  
6 Poetsch applied the MCC model with EGR corrections to a 5 cylinder, 2.5L Diesel engine [66] and tuned  
7 the model parameters over six engine operating points, however it is unclear how many test points  
8 (EGR rates, injection timings etc.) were used at each operating point.

9 For the phenomenological models built on the works of Barba, EGR effects are accounted for explicitly  
10 as the fraction of burnt gases influences the ignition delay and the equivalence ratio influences the  
11 diffusion combustion [50-53, 55, 56].

12 This study will apply a MCC model including several model correction factors to the full  
13 speed/load/EGR operating envelope of a 2.0L Diesel engine using only a small, but carefully selected,  
14 dataset for model training. A model built on the works of Chmela is chosen as it is mathematically  
15 simpler than the models based on the works of Barba [50] which is therefore more suited to the real-  
16 time requirement. The combustion model will be described; then the model parameterisation process  
17 will be detailed. Finally, the model performance will be assessed over the full engine operating range.

### 18 **3. Combustion model**

19 The combustion model is constructed as a combination of models proposed individually in the  
20 literature. Their combination is described in detail in the following section. The key novelty of this  
21 work lies in the use of a simple parameter for the incorporation of EGR that is parameterised using  
22 only a single EGR sweep at one engine operating condition, but that can extrapolate across the full  
23 EGR operating region. The model performance in extrapolation will be presented and analysed in  
24 detail in section 5.

### 3.1. Base Combustion model

The base heat release model considers separately the pre-mixed combustion and the diffusive combustion such that the total heat release is the sum of the two (equation 2).

$$\frac{dQ_c}{dt} = \frac{dQ_{pre}}{dt} + \frac{dQ_{diff}}{dt} \quad 2$$

The control volume is assumed to be a homogeneous mixture of gases at a single temperature and pressure and having the thermodynamic properties of the weighted average of the gas composition. With knowledge of each of the terms in the right-hand side of equation 1, the change in internal energy of the control volume can be estimated, if the charge behaves as a perfect gas. The heat loss at the cylinder walls was modelled using the work of Finol [67] with cylinder temperature imposed from measurements.

The premixed combustion is calculated using the build-up of fuel during the ignition delay (equation 3 [45, 47]) which includes:

- A term describing the reaction rate of the mixture
- An exponential term capturing the heating of the fuel
- The potential thermal energy available in injected fuel
- A quadratic term that captures the time elapsed since start of combustion to describe the initial burn rate.

$$\frac{dQ_{pre}}{dt} = a_1 \frac{\lambda \cdot AFR_{stoich}}{V_{mix}} e^{-a_2 \frac{T_a}{T_{cyl}}} m_{pre,avail}^2 LCV (t - t_{SOC})^2 \quad 3$$

$$where V_{mix} = m_{pre,avail} \left( \frac{1}{\rho_{f,vap}} + \frac{\lambda \cdot AFR_{stoich}}{\rho_{cyl}} \right)$$

1 The mean equivalence ratio in the mixture cloud,  $\lambda$ , is a model parameter that is assumed to be 0.5  
 2 for pre-mixed combustion for both main and pilot combustions.

3 Before the start of combustion, the mass of fuel that is available for pre-mixed combustion is  
 4 calculated as a proportion of the fuel injected into the cylinder, less the amount of fuel that may have  
 5 already burnt (during a previous injection). After the start of combustion, it is assumed that all  
 6 subsequent injected fuel burns in a diffusive mode (equation 4). The proportion of fuel dedicated to  
 7 the pre-mixed combustion,  $x_{pre}$ , was determined empirically but assumed to be constant for all  
 8 operating points.

$$m_{pre,avail} = \begin{cases} x_{pre} \int_{SOI}^{\theta} dm_{f,inj} - \frac{Q_{pre}(t)}{LCV} & \theta < \theta_{SOC} \\ 0 & \theta \geq \theta_{SOC} \end{cases} \quad 4$$

9  
 10 The amount of fuel contributing to the pre-mixed combustion is primarily determined by the ignition  
 11 delay period. This is the period after the start of injection but before the start of combustion. During  
 12 this period, the liquid fuel injected into the cylinder is mixed with surrounding cylinder charge,  
 13 evaporated, and heated up to its self-ignition temperature – this is termed the physical ignition delay.  
 14 Preliminary chemical reactions also occur during this period prior to ignition – this is represented by  
 15 the chemical ignition delay. Ignition is determined by the contribution of both these parameters  
 16 according to equation 5: start of combustion occurs when the integral term reaches unity [56].

$$\int_{SOI}^{SOC} \frac{1}{\tau_{ID}} dt = 1, \text{ where } \tau_{ID} = \tau_{ph} + \tau_{ch} \quad 5$$

17  
 18 The two delay terms are calculated according to the Arrhenius and Magnussen delay terms given in  
 19 equations 6 and 7 [45, 68, 69]. The chemical delay is linked to the ratio of temperature to activation  
 20 temperature which drives the chemical reactions. The physical delay is primarily driven by turbulence

1 in the cylinder which promotes the heating of the fuel. Both delay terms are scaled by a measure of  
 2 the concentration of fuel and oxygen.

$$\frac{1}{\tau_{ch}} = C_{arr} c_f c_o e^{-\frac{a_3 T_a}{T_{cyl}}} \quad 6$$

$$\frac{1}{\tau_{ph}} = C_{mag} c_f \frac{\sqrt{k}}{\sqrt[3]{V_{cyl}}} \quad 7$$

$$\text{where } c_f = \frac{m_f}{V_{mix}}, \quad c_o = \frac{0.232 m_{cyl}}{V_{mix}}$$

3  
 4 The diffusion combustion model is equivalent to the original MCC [42] (equation 8). The rate of heat  
 5 release is linked to the amount of fuel available for combustion and the rate of mixing, described  
 6 through an empirical turbulent kinetic energy term. This assumes that the turbulent energy comes  
 7 from the piston motion (engine speed) and the fuel injection. It also includes a factor for spray  
 8 impingement onto the cylinder wall [70].

$$\frac{dQ_{diff}}{dt} = C_{wall} \cdot C_{mod} \cdot LCV \cdot m_{f,diff,avail} \left( \frac{\sqrt{k}}{\sqrt[3]{V_{cyl}}} \right) \quad 8$$

9  
 10 The mass of fuel available for diffusive combustion is the mass of non-combusted fuel that has been  
 11 injected into the cylinder and that has evaporated as described by equation 9.

$$m_{f,diff,avail} = \int_{SOI}^{\theta} dm_{f,diff,vap} - \frac{Q_{diff}}{LCV} \quad 9$$

12  
 13 The evaporation rate of fuel is dependent on temperature, turbulent motion and droplet size and is  
 14 captured through equation 10.

$$\frac{dm_{f,diff,vap}}{d\theta} = \frac{1}{6N_{eng}} \int_{SOI}^{\theta} \frac{(T_{cyl})^{3.3} k}{C_{evap} d_{noz}} m_{f,diff,liqu} \quad 10$$

The turbulent energy density  $k$  is calculated from the turbulent energy caused by fuel injection and the energy dissipated within the cylinder as in [42].

The mass of liquid fuel available for evaporation is determined as the amount of fuel dedicated for diffusive combustion that has been injected into the cylinder but has not yet evaporated (equation 11).

$$m_{f,diff,liqu} = \begin{cases} (1 - x_{pre}) \int_{SOI}^{\theta} dm_{f,inj} - m_{f,diff,vap} & \theta < \theta_{SOC} \\ \left( (1 - x_{pre}) \int_{SOI}^{SOC} dm_{f,inj} + \int_{SOC}^{\theta} dm_{f,inj} \right) - m_{f,diff,vap} & \theta \geq \theta_{SOC} \end{cases} \quad 11$$

## 3.2. Extension to combustion model for EGR

### 3.2.1. Thermal Effect

The thermodynamic properties of the charge due to the displacement of oxygen by CO<sub>2</sub> and water account for the thermal effects of EGR (changes heat capacity). At any given point, the total cylinder mass is composed of a mixture of three species: fresh air, burnt gas and unburnt fuel. The thermodynamic properties of specific heats ( $C_p$ ,  $C_v$  and  $\gamma$ ) and specific internal energy ( $u$ ) each were calculated as a function of cylinder temperature [59]. The average thermodynamic properties of the cylinder were calculated by equation 12. The specific gas constant in the cylinder,  $R_{cyl}$ , was also calculated in this way taking gas constants for the air, fuel and burnt gases to be 287.05J/kgK [31], 55.95J/kgK and 285.4J/kgK [71] respectively.

$$c_{p,cyl} = Y_{air}c_{p,air} + Y_f c_{p,f} + Y_b c_{p,b}$$

12

$$\text{where } Y_{air} + Y_f + Y_b = 1$$

1  
2 The mass fraction terms,  $Y$ , are calculated based on the mass of the particular species and the total  
3 mass in the cylinder

$$Y_{air} = \frac{m_{air,cyl}}{m_{cyl}}, \quad Y_f = \frac{m_{f,cyl}}{m_{cyl}}, \quad Y_b = \frac{m_{b,cyl}}{m_{cyl}} \quad 13$$

4  
5 The composition of the cylinder when the intake valve closed was determined from the concentrations  
6 in the intake manifold and a filling and emptying model (see section 3.2.4). After intake valve closing,  
7 the masses of the individual components will evolve as follows:

- 8 - Fresh air mass will reduce as the air is burnt. In addition, any blow by flows or flows through  
9 the exhaust vale will also reduce the aim mass:

$$dm_{air,cyl} = -\frac{dQ_c}{LCV} (AFR_{stoich}) - Y_{air,cyl} (dm_{exh} + dm_{bb}) \quad 14$$

- 10  
11 - Fuel mass will increase at the rate at which it is injected into the cylinder, but reduce at the  
12 rate at which it is burnt:

$$dm_{f,cyl} = dm_{f,inj} - \frac{dQ_c}{LCV} \quad 15$$

- 13  
14 - Burnt gas mass will increase following the combustion of fuel and fresh air but reduce by any  
15 blow-by or exhaust valve flows:

$$dm_{b,cyl} = \frac{dQ_c}{LCV} (1 + AFR_{stoich}) - Y_{b,cyl} (dm_{exh} + dm_{bb}) \quad 16$$

At any point, the change in total mass in the cylinder is the sum of the change in air, fuel and burnt gas masses

$$dm_{cyl} = dm_{air,cyl} + dm_{f,cyl} + dm_{b,cyl} \quad 17$$

### 3.2.2. Dilution Effect

Both ignition delay, pre-mixed and diffusive combustion are affected by the mixing of injected fuel with the surrounding gases such that sufficient oxygen is available. The dilution effect of EGR reduces the availability of oxygen and therefore interferes with this process.

For ignition delay, closer inspection of the term  $c_o$  in equation 6 shows that the numerator represents the mass of oxygen in the cylinder. To account for the reduced oxygen in the cylinder, this should be augmented according to equation 18.

$$c_{o,EGR} = \frac{0.232m_{cyl}}{V_{mix}} (AFR_{stoich} (1 - \chi_{EGR})) \quad 18$$

Where  $\chi_{EGR}$  is the fraction of EGR by mass as defined in equation 24.

The dilution effect will also influence the pre-mixed combustion by affecting the propagation of the flame front and the diffusion combustion because more gas must be mixed into the combustion flame increasing its volume. Equations 3 and 8 are therefore modified into equations 19 and 20 respectively to account for these effects [46, 48].

$$\frac{dQ_{pre}}{dt} = a_1 \frac{\lambda \cdot AFR_{stoich}}{V_{mix}} e^{-a_2 \frac{T_a}{T_{cyl}}} m_{pre,avail}^2 LCV (t - t_{SOC})^2 (1 - \chi_{EGR})^{a_4} \quad 19$$

$$\frac{dQ_{diff}}{dt} = C_{mod} \cdot LCV \cdot m_{f,diff,avail} \left( \frac{\sqrt{k}}{\sqrt[3]{V_{cyl}}} \right) (1 - \chi_{EGR}) \quad 20$$

### 3.2.3. Chemical effect

The chemical effect of EGR is considered only minor and difficult to implement in a single zone model where only average cylinder temperature is calculated as the dissociation reactions rely on peak local cylinder temperatures. Considering the real-time nature of the proposed heat release model, these parameters are ignored.

### 3.2.4. Modelling external flow of EGR

Although this work considers only the effects of EGR on the combustion heat release in the cylinder, the external flow of EGR is an important parameter as it affects the composition of the gas when the intake valve closes. The EGR layout for the engine in this study is shown in Figure 3. This was modelled by considering four control volumes: the cylinder, intake and exhaust manifolds, and the EGR cooler. [72]. It is important to note that the model includes experimentally validated models for:

- Exhaust manifold heat transfer was calculated by forced convection using the Nusselt/Reynolds correlation [73] and an empirical wall temperature model.
- EGR Valve flow coefficient was captured by an empirical quadratic function expressing effective valve area to valve lift.
- EGR cooler effectiveness was mapped as a function of EGR mass flow rate based on measured gas temperatures.



## 4. Experimental Approach

### 4.1. Engine installation and operating points

Experiments were conducted on a 2.0L turbocharged, common rail Diesel engine installed on a transient engine dynamometer. A summary of the engine specification is given in Table 1. After the warm up phase of 20 minutes at mid-speed, mid-load to ensure that engine coolant and oil were at stabilised temperatures, the engine was taken to each steady-state speed/torque operating point as detailed in Figure 4. At each point the engine was held for a settling period of 5 minutes before recording operating data – this was required to achieve thermal stability at the operating point in question. For tests without EGR, low frequency data was recorded for a period of 30seconds and in-cylinder data was measured over 100 consecutive engine cycles. Diesel combustion, especially in the absence of EGR, is very stable unlike petrol combustion which justifies the low number of cycles. When EGR is introduced, combustion stability decreases because the recirculation of exhaust gases cause interactions between subsequent combustion cycles. With high levels of EGR, the standard deviation of pressure during combustion can increase by a factor of 2.5 [66]. To account for this, the number of combustion cycles recorded was increased to 300 for the tests with EGR.

**Table 1 - Specification of the 2.0L Diesel Engine**

Engine Type	Turbocharged diesel
Cylinders	4
Capacity	1998cc
Stroke	86mm
Bore	86mm
Conrod Length	152mm
Firing Order	1-3-4-2
Compression Ratio	16
Max Torque	320Nm at 1800-2000rpm
Max Power	95kW at 3800rpm
Fuel Injection	Common rail direct injection up to 1600bar

1 For every point the engine map in Figure 4, data was captured with no external EGR flow. Figure 4 also  
2 highlights the sub-region of the engine operating map where EGR tests were conducted. For points  
3 within the EGR test region, measurements were taken at different EGR rates, varied in five equal steps  
4 between no EGR and the maximum EGR rate at that point. Whilst undertaking each of the EGR rate  
5 sweeps, fuel injection quantity and fuel injection timing were maintained constant. As the EGR valve  
6 was opened, changes in boost pressure were compensated for by adjusting the variable geometry  
7 turbocharger guide vane angle – this delivers EGR by reducing the fresh air charge. Figure 5 shows the  
8 maximum EGR rate that can be achieved within the EGR region. The maximum EGR rate was  
9 determined based on the effect of EGR on Hydrocarbon (HC) and carbon monoxide (CO) emissions:  
10 the limiting EGR rate was determined as the point at which HC or CO had increased by more than  
11 300% compared to the zero EGR case or the point at which EGR flow could not be increased without  
12 a drop in intake manifold pressure. Points in Figure 4 without EGR were also identified by the same  
13 criteria.

#### 14 **4.2. Instrumentation and measurements**

15 The engine was monitored by two data acquisition systems: the first was a *CP Engineering Cadet*  
16 *Automation System* monitoring low frequency data at a rate of 20Hz and the second was a *D2T Osiris*  
17 system capturing indication data for every 0.1°CA. Table 2 summarizes the key instrumentation used  
18 in this study.

1

**Table 2: Summary of key Instrumentation sensors**

Low frequency		CP Engineering Cadet Automation system	
Channel	Sensor	Range	Accuracy
Fuel Flow	CP FMS1000 Gravimetric Flow Meter	0-300kg/h	+/-0.05% <sup>(a)</sup>
Air Flow	ABB Sensy flow FMT700-P hot wire flow meter	0-800kg/h	+/-1%
Gas Pressure	Piezo-resistive pressure transducers	0-5bar <sup>(b)</sup>	+/-10kPa
Gas Temperature	k-type thermocouple 1.5mm	0-1200K	+/-2.2°C
Engine Torque	HBM analogue torque sensor	-500-500Nm	0.05%
CO <sub>2</sub> Emissions concentrations	Horiba Mexa 7000 Analyser	0.5-20%vol	2% <sup>(c)</sup>

High Frequency		D2T Osiris System	
Channel	Sensor	Range	Accuracy
In-cylinder pressure	Kistler Piezoelectric Pressure Sensor (Type 6056A) installed in glow plug adaptor	0-250bar	+/-2% <sup>(d)</sup>
Fuel rail pressure	Kistler Piezoelectric Pressure sensor (Type 4067A) installed on rail supply pipe	0-2000bar	+/-0.5%
Injector current	Pico Technology TA009 current clamp	10mA-20A	+/-2%+/-5mA

(a) Does not include installation effects which can affect the accuracy of measuring fuel consumed using gravimetric flow meters [74]

(b) Range of pressure transducers used to measure intake manifold and exhaust manifold pressures.

(c) Emissions analyser accuracy achievable with daily calibration

(d) Accuracy for in-cylinder pressure measurement does not include the accuracy of pressure pegging (i.e. determining absolute values). This accuracy is the accuracy of the sensor which measures change in pressure over time and includes drift due to thermal shock

The EGR rate was determined by two measurements of CO<sub>2</sub> volumetric concentration, the first taken in the exhaust flow ( $CO_{2,exh}$ ) just after the turbocharger turbine and the second taken from the intake manifold ( $CO_{2,int}$ ). Both volumetric concentrations are converted into mass concentrations according to equation 21.

$$Y_{CO_2,i} = \frac{\dot{m}_{CO_2,i}}{\dot{m}_i} = K_{dw} u_{CO_2} C_{CO_2,i} \quad 21$$

Where  $C_{CO_2}$  is a volumetric concentration measured by the emissions analysers,  $i$  represents either inlet of exhaust manifolds,  $u_{CO_2}$  is a constant and  $K_{dw}$  is a correction factor to account for the fact that the emissions analyser removes water vapour before measuring the CO volumetric concentration [75].

1 EGR mass airflow was calculated by applying a CO<sub>2</sub> balance as shown in equation

$$(\dot{m}_{air} + \dot{m}_{EGR})Y_{CO_2,inl} = \dot{m}_{air}Y_{CO_2,air} + \dot{m}_{EGR}Y_{CO_2,exh} \quad 22$$

2  
3 Assuming the CO<sub>2</sub> concentration in the fresh intake air,  $Y_{CO_2,air}$ , is negligible, then the EGR mass flow  
4 can be obtained from the two CO<sub>2</sub> concentrations and the measured intake air flow according to  
5 equation 22.

$$\dot{m}_{EGR} = \frac{Y_{CO_2,inl}\dot{m}_{air}}{Y_{CO_2,exh} - Y_{CO_2,inl}} \quad 23$$

6 EGR fraction can then be found as a function of  $\dot{m}_{EGR}$  and  $\dot{m}_{air}$ , as show in equation 24.

$$\chi_{EGR} = \frac{\dot{m}_{EGR}}{\dot{m}_{air} + \dot{m}_{EGR}} \quad 24$$

### 7 **4.3. Determining Measured Combustion Parameters**

8 Measured indicated data was pre-processed to allow comparison model. Raw pressure data was  
9 collected for 100 consecutive engine cycles and the following data processing steps were taken before  
10 computing the combustion parameters:

- 11 - An angle based arithmetic average of the 100 cycles was calculated to remove random noise.
- 12 - A double-spline low-pass filter [76] was applied to smooth systematic noise in the pressure  
13 trace. This noise largely consists of high frequency pressure oscillations caused by the high  
14 rate of pressure rise during pre-mixed combustion, but also includes noise caused by the inlet  
15 and exhaust valve movements.
- 16 - The absolute magnitude of pressure was pegged by assuming the pressure rise during  
17 compression to be polytropic and using the two-point method with fixed polytropic index [77].

- 1           - The measured pressure trace was aligned with the calculated cylinder volume by identifying  
2           the location of top dead centre through a motored pressure trace and inclusion of  
3           thermodynamic offset [78].

4           The raw pressure trace was subsequently used to calculate the observed combustion rate of heat  
5           release based on equation 1. In this analysis, the combustion heat release curve is the unknown with  
6           each of the other terms being known or modelled as follows:

- 7           - The internal energy term was estimated from the in-cylinder temperature, calculated from  
8           the measured cylinder pressure and the perfect gas law. The in-cylinder trapped mass was  
9           estimated using a filling and emptying model, the rate of fuel injection and blow-by [79]. For  
10          heat release calculation, the fuel injection rate was assumed to be constant for the injection  
11          duration and vaporization was ignored. Blow-by flow was estimated as an isentropic  
12          discharger through a nozzle [44]. The cumulative blow-by estimated by this model was  
13          validated using a Labcell M400MR Bow-By Monitor (accuracy +/-1.5%).
- 14          - The heat transfer term was modelled using the model proposed by Finol [70]
- 15          - The work term is calculated from the in-cylinder pressure and calculated cylinder volume [31].
- 16          - The intake and exhaust enthalpies were calculated based on the filling and emptying model  
17          and the in-cylinder temperature [80] and the blow-by enthalpy from blow-by flow using  
18          instantaneous nozzle model [71].

19          Using the processed in-cylinder pressure measurement, the calculated rate of heat release and a  
20          measurement of cylinder pressure from a motored cycle, the following quantities were calculated as  
21          followed:

22          Ignition delay was calculated as the time between start of injection and start of combustion. Start of  
23          injection was estimated based on measured current in the injector solenoid and a model of the  
24          injector hydraulics to account for needle lift delay. Start of combustion was determined differently for  
25          pilot and main injections:

- For pilot injection was determined by considering the second differential of in-cylinder pressure [68, 81]
- For main injection was determined by assessing when the calculated rate of heat release increased above a significant threshold. For high loads where pilot and main combustion overlap, a Wiebe model was fitted to the main combustion event to predict the start of main combustion.

Peak heat release rate, angle of peak heat release, peak pressure and angle of peak pressure were identified directly from the calculated heat release rates and processed pressures. The detailed uncertainty of each of these parameters is a complex topic and the focus of research in its own right, however a detailed sensitivity analysis performed by the authors has estimated the parameter accuracies in Table 3.

**Table 3: Estimated combustion metric measurement accuracy [75]**

<b>Output</b>	<b><i>IMEP</i></b>	<b><i>dQ<sub>c,max</sub></i></b>	<b><i>Q<sub>c</sub></i></b>	<b><i>SOC</i></b>	<b><i>Q<sub>HT</sub></i></b>
<b>Predicted error</b>	±1.1%	±4.9%	±1.4%	±0.29°CA	±12.2%

#### **4.4. Model Parameterisation**

For the simulation of all operating points, measured pressures in the intake and exhaust manifolds were imposed as well as measured temperature of the fresh air at the intercooler outlet (prior to mixing with the EGR flow). The cylinder wall temperature was also imposed based on cylinder temperature measurements [82]. For each condition, the simulated EGR valve opening was determined to match the measured cycle-averaged the fresh air flow.

The model was fitted using a single set of model parameters applied to all engine operating points. The parameterisation of the model was undertaken in a series of sequential steps which are detailed in figure 6. For each step in the identification, the targets model coefficients are highlighted from the model equations described in section 3. The experimental points used for the identification are also

1 shown and refer to the points in figure 4. The ignition delay can be measured directly from the in-  
2 cylinder pressure and the model prediction of ignition delay is not dependent on any other  
3 combustion sub-models; therefore, this model was parameterised first. A manual adjustment of the  
4 parameters was then necessary to achieve a sensible model output. This manual adjustment was  
5 based on information available in the literature and a trial and error approach. The next three steps  
6 provided the fine tuning of parameters for the diffusion and pre-mixed combustion. This process was  
7 performed iteratively as each model will influence the other when comparing the ability to match the  
8 measured rate of heat release. This iterative process was performed at operating points where wall  
9 impingement was unlikely and EGR was disabled. The final two steps then corresponded to the wall  
10 impingement and EGR model training.

11 Optimization of the model parameters was performed using the MATLAB algorithm '*fminsearch*',  
12 which minimizes the target function for a given set of coefficients. The optimisation target was  
13 different depending on the step in figure 6. The stopping criteria for the fitting algorithm was a  
14 convergence criterion whereby the model fit did not improve by more than a minimum threshold with  
15 each loop.

## 17 **5. Results and discussion**

18 Table 4 summarises the correlations of measured and modelled combustion parameters for test  
19 points with and without EGR. Most of the fit statistics without EGR have an  $R^2$  value in the region of  
20 0.99. In section 5.1 these results will be explored in more details, analysing the fit over the engine  
21 operating range. For tests with EGR, the model performs well in predicting in-cylinder pressure but  
22 struggles with the combustion metrics. In section 5.2 these results will be explored in further detail to  
23 understand the observed model performance.

24 **Table 4 – Comparison of model correlation coefficients ( $R^2$ ) for RoHR data with EGR, and without EGR**

Parameter	Without EGR	With EGR
$p_{max}$	0.989	0.946
$\theta_{max, RoHR}$	0.744	0.516
$\theta_{SOC, main}$	0.998	0.768
$RoHR_{max}$	0.961	0.323
$IME P_{gross}$	0.996	0.990

## 5.1. Base Combustion model without EGR

### 5.1.1. Rate of heat release prediction

Figure 7 compared measured and modelled rate of heat release for 12 different engine operating points without EGR. The model can capture both shape and magnitudes and the strongest points are:

1. Ignition delay and its effect on initial pre-mixed for operating points with a large proportion of pre-mixed combustion (points a, b and e).
2. Combustion decay after the end of injection - these are high load points with long injection durations and significant diffuse combustion (points g, h, k and l).
3. The end of combustion for low load points where the combustion is mainly pre-mixed and the end of combustion is dominated by the dynamics of the flame front (points a to d).
4. The effects of wall impingement which reduce peak heat release rates at full load conditions (points i to l).
5. The magnitude and phasing of pilot combustion for most operating points.

Weaker model performance was observed for the following conditions:

1. Pre-mixed combustion at high engine speeds (points d, h and l) which could have been caused by using a low speed operating point to parameterise the pre-mixed combustion model
2. Pilot combustion at where pilot quantity is small (points d, h and j), as a result the main combustion appears greater because fuel injected during the pilot injection is added to the fuel at the onset of combustion.



### 5.1.2. Ignition Delay

Figure 8 compares measured and predicted ignition delay for the main injection event. The graphs are grouped by engine speed and plotted against rail pressure which captures the increase in indicated torque, therefore higher rail pressure in this representation corresponds approximately to higher engine load. The ignition delay model, which is also affected by pilot injection and ignition, performs well for speeds above 2000rev/min (Figure 8 c to f). The model is worse at lower engine speeds and most markedly at 1000rpm (Figure 8a). This is the most challenging point for the cylinder filling and emptying model which leads to poor estimation of in-cylinder mass, pressure and crucially temperature. An underestimation of the cylinder temperature would cause the over-estimation of ignition delay. There is also more uncertainty in the measured start of combustion at highest and lowest speeds and low engine loads because it becomes difficult to distinguish between the main and pilot burn.

### 5.1.3. Peak Heat Release

The measured and modelled maximum heat release rates are compared on figure 9. The peak heat release rate increases with BMEP at all engine speeds and this trend and magnitude is correctly captured. The poorest agreement occurs at 3500rpm where there is an underestimate in overall magnitude.

### 5.1.4. Point of peak heat release

Figure 10 compares measured and modelled angle of peak in-cylinder pressure. Despite the low  $R^2$  value in table 4, the model qualitatively captures the trends and magnitudes, including the discontinuities between low and high loads at 1500rpm and 2500rpm. The most notable exception is at low load condition at 3000rpm (figure 10e). Considering the detailed plot of heat release rate for low load at 3000rev/min in figure 7c, this is explained by an overestimation of main combustion heat release rate.

## 5.2. Extended combustion model with EGR

### 5.2.1. Ignition delay

Figure 11 shows experimental and simulated ignition delay for the main injection. The model correctly predicts the trend of increased ignition delay with increased EGR rate. The model also reflects the interactions with engine speed and load which reduce the effect of EGR due to higher magnitudes of fresh air flow and fuel energy. One notable exception is the condition at 1500rpm and 100Nm where the model substantially over-predicts the impact of EGR due to the under-prediction of cylinder pressure and temperature prior to the main combustion event.

In many of the test points there is an offset between the experimental and predicted data, even for low EGR rates. This suggests that this error is not a response to the EGR modelling, but rather to another variable that affects the ignition delay sub-model. Small errors in-cylinder mass and temperature can have a large influence on ignition delay, and it is likely that assumptions made in the filling and emptying model and the heat transfer model will contribute to overall error. Mixing within the inlet manifold was assumed to be perfect, and cylinder-to-cylinder variations were ignored. In addition, cycle-to-cycle variation will result in discrepancies between time-averaged and cycle-averaged data, both of which are model inputs and model validation metrics.

The prediction of pilot affects pressure and temperature history prior to main injection and influences main injection ignition delay. In several cases, pilot combustion was over-predicted by up to 300%: Figure 12 shows an example of such a case. Overestimating the pilot combustion affects the main combustion in two ways:

- The temperature and pressure in the cylinder are higher (more energy release). This tends to shorten the ignition delay for the main injection as per equation 6. The shorter ignition delay leads to less fuel combusting in the pre-mixed mode
- There is less unburned fuel, injected but not burnt during the pilot injection that will subsequently burn in the main combustion event.

1 The difference in pilot prediction is thought to be due to the very early injection timing employed  
2 when EGR is enabled. It is hypothesised that this leads to the pilot combustion leaning out due to  
3 excess air before all the fuel has been consumed, since this was observed even with very low  
4 concentrations of EGR. The ignition delay for main injection would increase because the temperature  
5 rise from pilot injection is reduced and it is possible that the unburnt fuel from the pilot then  
6 contributes to the main combustion event. Both will increase the main pre-mixed spike as seen in the  
7 measured data (see Figure 12). Since the model assumes a fixed stoichiometric ratio ( $\lambda$ ) for pilot  
8 combustion, it is not possible for the current simulation to model this behaviour. In addition, the effect  
9 of EGR on pilot combustion would be magnified compared to the effect on main combustion due to  
10 small amount of fuel and long ignition delay, reducing peak heat release rates further.

### 11 **5.2.2. Peak RoHR**

12 Figure 13 compares modelled and measured maximum heat release rate for different EGR rates and  
13 speed load points. Overall, the prediction for peak heat release rate is relatively poor compared to the  
14 other combustion metrics. This is especially true for low loads where there are large offsets between  
15 the measured and predicted data. For medium to high loads, the model offers better prediction.  
16 However, at these test points, the effect of EGR is reduced significantly because the EGR rates are  
17 lower and the charge densities higher.

18 This split between low-load and high-load conditions can be explained by the dominance of pre-mixed  
19 combustion. At low loads a greater portion of the fuel mass is dedicated to the pre-mixed model, since  
20 there is significantly more ignition delay at this point. This effect is amplified by the presence of EGR,  
21 which retards the SOC further and increases the pre-mixed portion. Although the trend in ignition  
22 delay was predicted well, there were significant offsets between the predicted and measured data  
23 (Figure 11). At low loads, the peak heat release rate is very sensitive to the amount of fuel dedicated  
24 to the pre-mixed model, and therefore also to the ignition delay: small errors in ignition delay can  
25 cause a large model errors. In some cases, it appears as if there is a greater amount of pre-mixed

1 combustion than would be predicted, even if the model predicted the SOC correctly. In these cases, it  
2 is theorised that a greater fraction of fuel injected during the ignition delay should have been  
3 dedicated to the pre-mixed combustion model, due to the presence of EGR and partially burnt pilot.  
4 Detailed assessment of the model presented by Rether et al. [39] shows the inclusion of varying excess  
5 air ratio during the pilot injection could improve the simulation at low load.

### 6 **5.2.3. Point of peak RoHR**

7 The point of peak RoHR ( $\theta_{max,RoHR}$ ) is a useful metric of combustion phasing because it is a function  
8 of both ignition delay and RoHR. These results are plotted in figure 14. The trend of  $\theta_{max,RoHR}$   
9 increasing with additional EGR is predicted well by the model. In addition, the magnitude of  $\theta_{max,RoHR}$   
10 is predicted well with some offsets observed particularly around mid-load points. In most cases, the  
11 offsets can be attributed to poor ignition delay prediction; however, the results for 2500rpm and  
12 3000rpm, 100Nm load can be attributed to the model not predicting diffusion combustion correctly.

13 Figure 15 shows an example of early prediction of peak RoHR: the measured data clearly exhibits two  
14 distinct peaks; the first being the pre-mixed event, and the second the peak diffusion event. The RoHR  
15 prediction is reasonable up to the first peak, showing that the differences can be attributed to the  
16 diffusion model. In the model, the RoHR is proportional to the available fuel mass and rate of injection,  
17 so at the EOI there is an exponential decay in RoHR. What this data implies is that either the rate of  
18 injection is over-predicted for this test point, or that there is another mechanism which is delaying the  
19 diffusion burn. It was assumed that the time for the fuel to reach the flame sheet was negligible, and  
20 that the kinetic energy density is proportional to the needle lift. In [46], it was suggested that there  
21 should be a time lag proportional to the injection rate to account for the time for fuel energy to reach  
22 the flame sheet. Since EGR increases the injection delay, and combustion occurs over an increased  
23 volume, the diffusion flame sheet is further away from the injector. This means the time delay  
24 becomes more significant, resulting in the phenomenon observed. The low  $R^2$  for  $\theta_{max,RoHR}$   
25 presented in table 4 could have been caused by operating point offsets, which were due to poor SOC

1 prediction, since the trends with increasing EGR rate appear to be captured as explained in Section  
2 5.2.3.

### 3 **5.3. Summary of future model improvements**

4 The shortfalls of the model with respect to EGR have been touched upon through the results analysis.  
5 These relate to all three of the combustion phases: pilot, pre-mixed and diffusion. The results  
6 suggested that pilot combustion was overpredicted when with the presence of EGR and this suggests  
7 that the influence of EGR on the pilot model should be increased. In particular, the model needs to be  
8 more sensitive to temperature and mixing and to have the ability stop the pilot combustion. This could  
9 be achieved by tuning the stoichiometric ratio ( $\lambda$  in equation 3) without EGR and whilst it offers  
10 simplicity, data from the EGR tests could be used to add mathematical flexibility to improve the  
11 prediction.

12 In some operating points the premixed combustion is underestimated with EGR. This problem could  
13 be solved by adjusting the amount of fuel partaking in the premixed combustion phase. This could  
14 either be achieved by varying the stoichiometric ratio for premixed combustion ( $\lambda$  in equation 3) or  
15 the amount of fuel dedicated to premix combustion ( $x_{pre}$  in equation 4). As for pilot, these two terms  
16 were parameterised without EGR and maintained constant for all operating points. Some dependency  
17 on EGR could be introduced to these terms. This would again increase the complexity of the model in  
18 exchange for potential benefits in accuracy.

19 For the diffusion combustion, a time lag to account for the fuel reaching the flame sheet could be  
20 added. This would need to be incorporated in the expression for  $m_{f,diff,avail}$  (equation 9). In practice,  
21 this time lag would be a function of the velocity of the fuel injected into the cylinder (linked to rail  
22 pressure) and the size of the flame. As the flame will be larger in the presence of EGR, this term could  
23 be set as a function of EGR rate or in-cylinder concentration.

24 Each of these proposed model modifications would increase the number of parameters that need to  
25 be identified and therefore increase the empirical aspects of the model. Ultimately each individual

1 application would need to trade-off this aspect depending on the available training data and modelling  
2 targets.

## 3 **6. Conclusions**

4 A Mixed Controlled Combustion model had been presented including enhancements for wall  
5 impingement, pre-mixed combustion, pilot combustion and EGR. The model was parameterised using  
6 a small set of selected engine operating points. Initially the combustion model parameters were  
7 identified without EGR and the resulting model predicted Rate of heat release, start of combustion,  
8 peak pressure, and combustion phasing with  $R^2$  values above 0.95 across the complete engine  
9 operating map.

10 From the base model, the EGR parameters were identified using specific EGR test points and validated  
11 using measured EGR swings over the engine's EGR operating envelope. The  $R^2$  values comparing  
12 simulation and measured results for the same combustion parameters were all reduced over the EGR  
13 operating region. However, close examination of results shows that most trends were captured well.  
14 Key errors in the pilot combustion were identified that have knock on effect onto the main combustion  
15 phasing and peak rates. However, despite these differences, the in-cylinder pressure was well  
16 predicted.

17 Pilot combustion was found to be over-predicted, since the pilot timing was early compared to  
18 conditions without EGR, resulting in pilot combustion leaning out and contributing to the main  
19 combustion. A more complex pilot model which considers the pilot  $\lambda$  to be variable, and could pass  
20 fuel between the pilot and main combustion models, would be required to simulate this effect  
21 accurately.

22 Peak heat release prediction was found to be relatively poor; however, this was mainly due to large  
23 offsets observed at the constant speed/load test points, rather than the correlation with change in  
24 EGR rate. Peak rates were affected, especially at low loads where combustion is mainly pre-mixed and  
25 most reliant on the SOC being correct, since SOC defines the portion of fuel dedicated to the pre-

1 mixed model. Also, it is suggested that partially burnt pilot may have contributed to the increased heat  
 2 release rates during the initial pre-mixed burnt at low loads.

### 3 7. Notation

$AFR_{stoich}$	Stoichiometric air fuel ratio	
$a_{1-4}$	Model fitted parameters	
$C_{arr}$	Arrhenius model constant (Fitted)	
$C_{CO_2}$	Volumetric concentration of CO <sub>2</sub>	%
$C_{evap}$	Fuel Evaporation model constant	
$C_{mag}$	Magnussen model constant (Fitted)	
$C_{mod}$	Chmela diffusion Combustion model constant (fitted)	J/kg °CA
$C_p$	Specific heat capacity at constant pressure	J/kgK
$C_V$	Specific heat capacity at constant volume	J/kgK
$d_{noz}$	Injector Nozzle diameter	m
$IMEP_{gross}$	Gross Indicated mean effective pressure	Pa
$H$	Enthalpy	J
$h$	Specific enthalpy	J/kg
$K_{dw}$	Dry/wet correction factor for CO <sub>2</sub> emissions measurement	
$k$	Turbulence density	m <sup>2</sup> /s <sup>2</sup>
$LCV$	Lower Calorific Value of fuel	J/kg
$m$	mass	Kg
$N_{eng}$	Engine Speed	Rev/min

$p$	pressure	Pa
$Q_C$	Heat energy from combustion	J
$Q_{HT}$	Heat transfer through cylinder walls	J
$R$	Gas constant	J/kgK
$R^2$	Coefficient of Determination	
$SOC$	Start of Combustion	°ATDC
$T$	Temperature	K
$T_a$	Fuel Activation Temperature	K
$t$	time	s
$U$	Internal energy	J
$u_{CO2}$	Relative density constant for CO2 emissions measurement	
$V$	Volume	m <sup>3</sup>
$W$	Work	J
$x$	Proportion of fuel	
$Y$	Mass fraction	
$\gamma$	Ratio of specific heats	
$\theta$	Crank Angle	°
$\lambda$	Stoichiometric ratio for premixed combustion	
$\rho$	density	Kg/m <sup>3</sup>
$\tau$	Delay time constant	s <sup>-1</sup>
$\chi_{EGR}$	Fraction of EGR by mass	



<i>air</i>	Fresh air
<i>avail</i>	Available fuel
<i>b</i>	Burnt gases
<i>bb</i>	Blow-by flow
<i>CO<sub>2</sub></i>	Carbon Dioxide
<i>ch</i>	Chemical Ignition delay
<i>diff</i>	Diffusive combustion
<i>cyl</i>	In-cylinder
<i>EGR</i>	Exhaust gas recirculation
<i>exh</i>	Flow through exhaust valves
<i>f</i>	fuel
<i>ID</i>	Ignition Delay
<i>inj</i>	Injected
<i>inl</i>	Flow through intake valves
<i>liqu</i>	Liquid
<i>main</i>	Main injection or combustion event
<i>max</i>	Peak/maximum
<i>ph</i>	Physical ignition delay
<i>pre</i>	Pre-mixed combustion
<i>soc</i>	Start of combustion
<i>SOI</i>	Start of Injection

*vap*      evaporated

1

ATDC      After top dead centre

BMEP      Brake Mean Effective Pressure

CA      Crank Angle

CO<sub>2</sub>      Carbon dioxide

EOI      End of Injection

HiL      Hardware in the Loop

MCC      Mixing Controlled Combustion

NO<sub>x</sub>      Oxides of nitrogen

RoHR      Rate of Heat Release

SOC      Start of Combustion

SOI      Start of Injection

SSE      Sum Squared Error

TDC      Top dead centre

2

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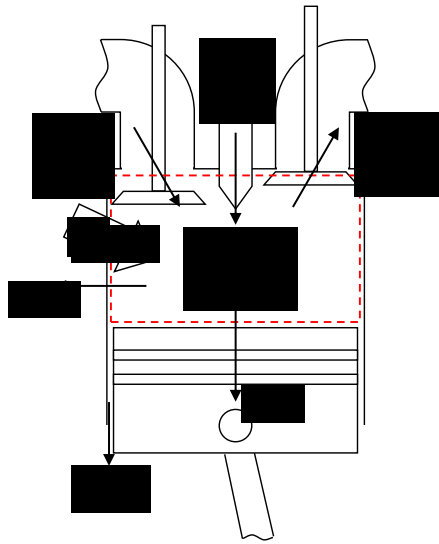
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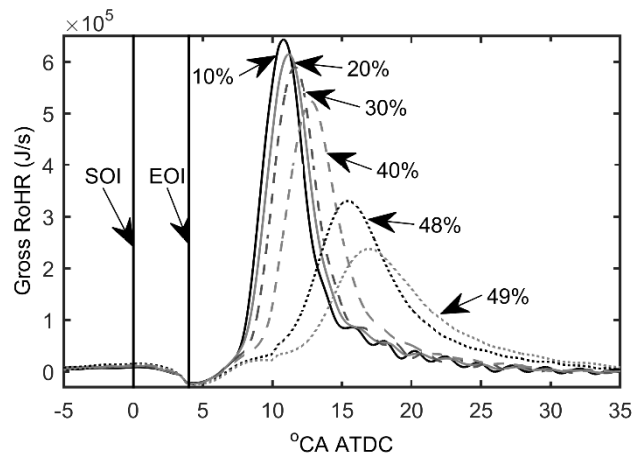


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1  
2 **Figure 1: Combustion chamber control volume with mass and energy transfer for a single zone model**



3  
4 **Figure 2: Effect of increasing percentage EGR on apparent heat release at 2000rev/min and 20Nm**

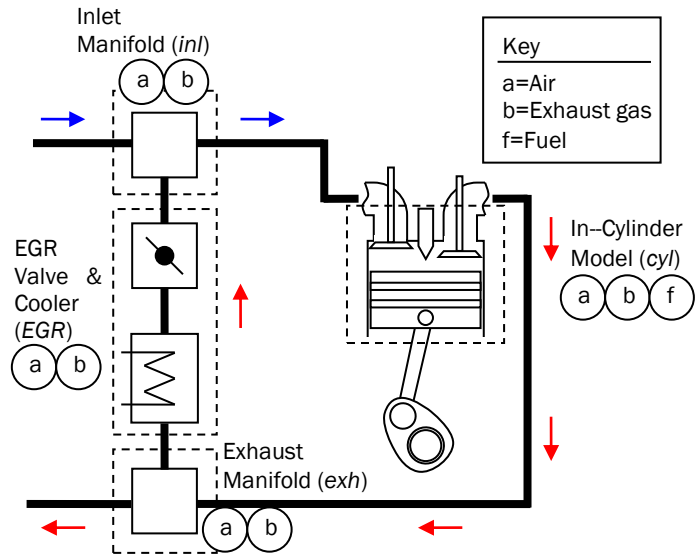


Figure 3: Layout of control volumes for air path model to estimate flows of EGR and cylinder gas composition

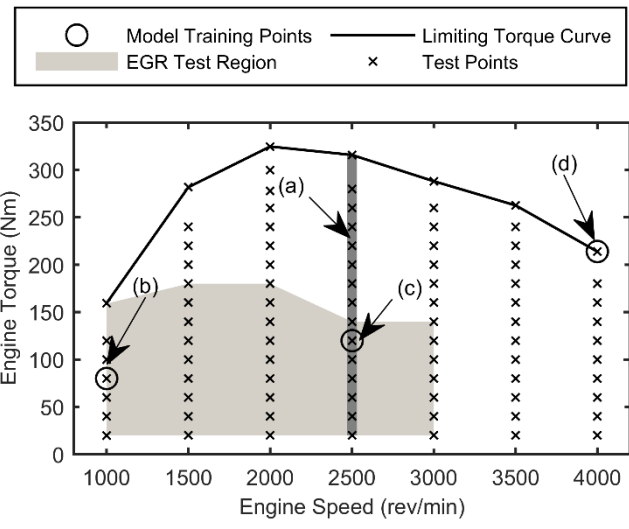


Figure 4: Engine speed/ torque map illustrating all test points used for model validation. Points used for model training are highlighted as: (a) diffusion combustion, (b) pre-mixed combustion, (c) ignition delay and (d) wall impingement

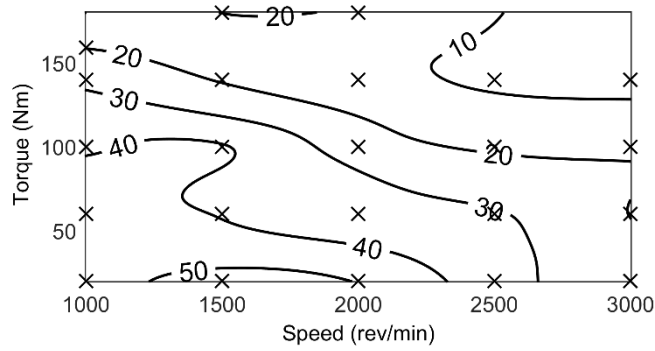
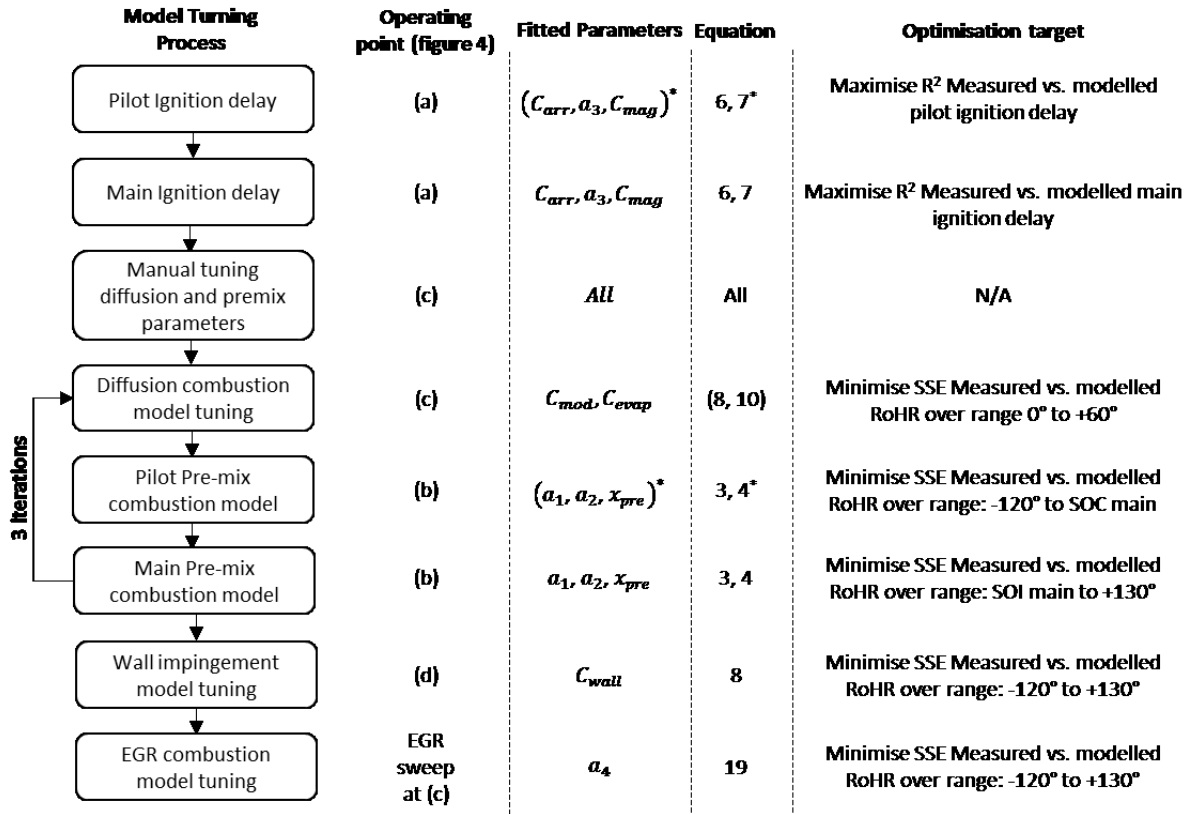


Figure 5: Maximum achievable EGR rates within the EGR test region



\*indicates dedicated model coefficients for the pilot injection

RoHR: Rate of Heat Release

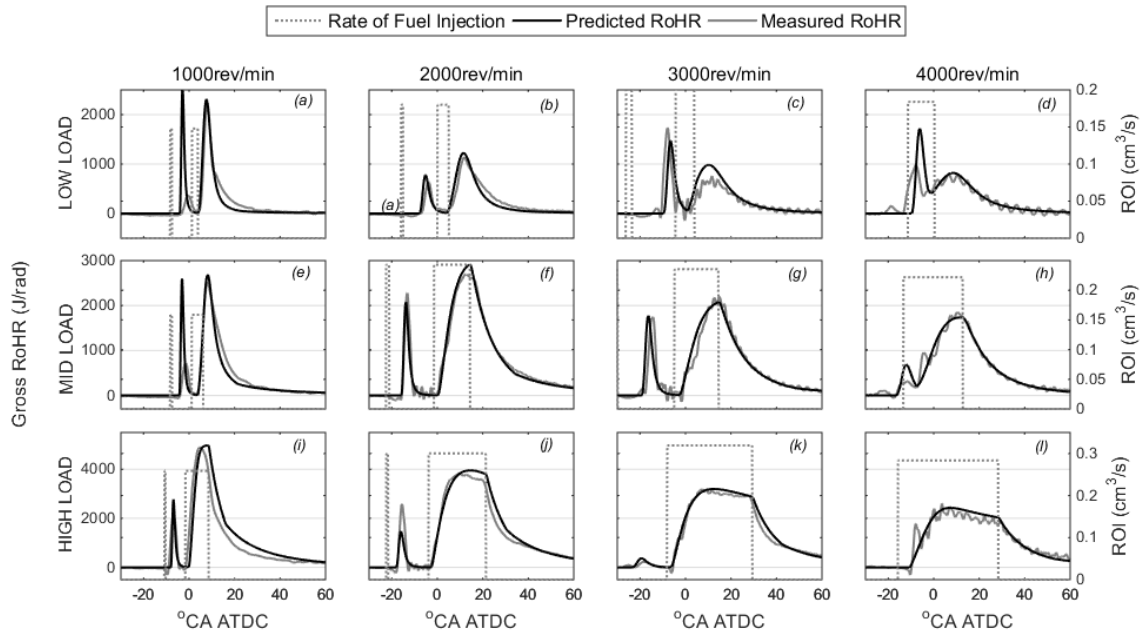
SSE: Sum Squared of errors

$R^2$ : Coefficient of determination

SOI: Start of injection

SOC: Start of combustion

Figure 6: Model parameter training process



1  
2 **Figure 7: Rate of injection and predicted and measured gross heat release rate for a range of engine**  
3 **speeds and loads without EGR**  
4

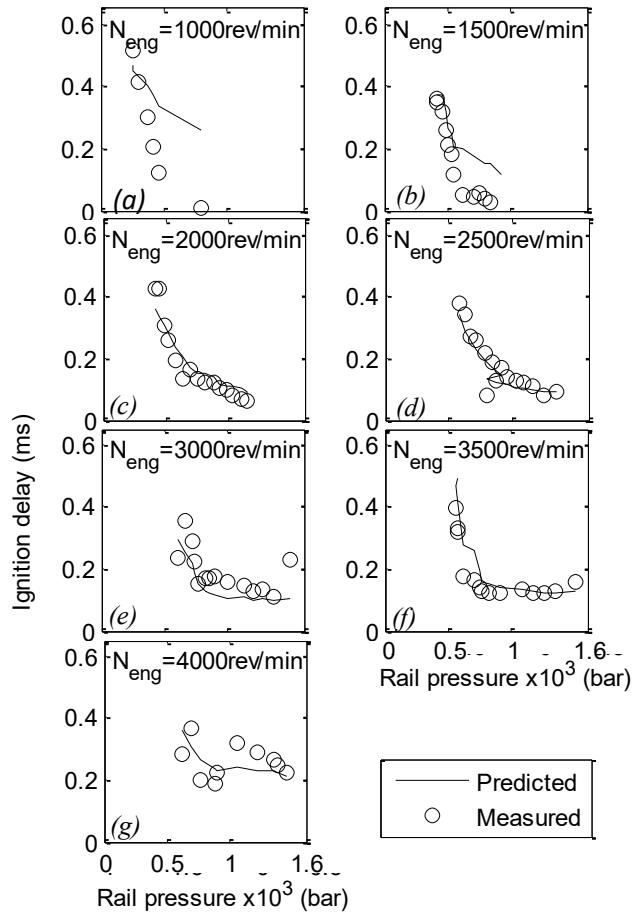


Figure 8: Measured and predicted main injection ignition delay grouped by operating speeds

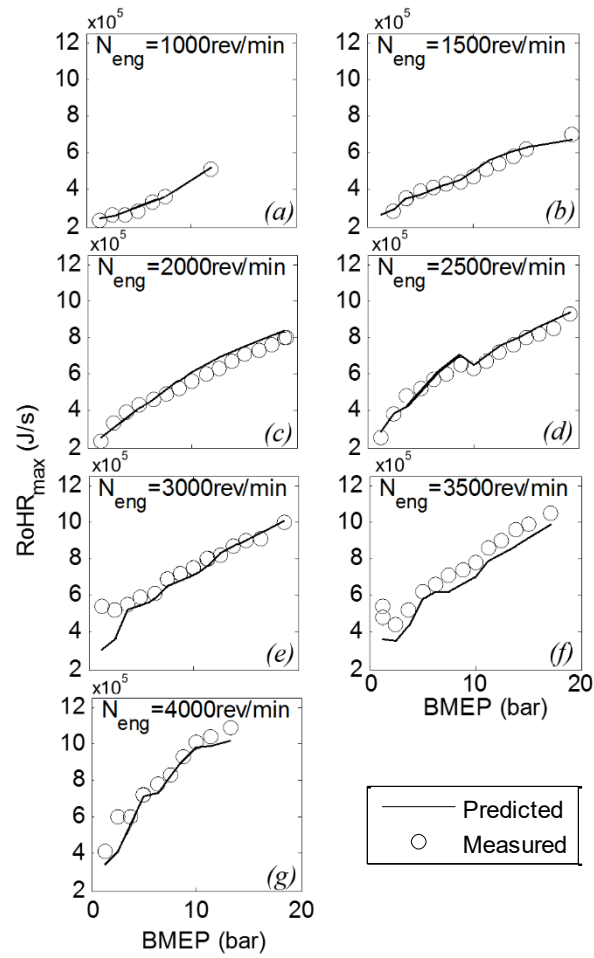


Figure 9: Measured and predicted peak heat release rate grouped by operating speeds



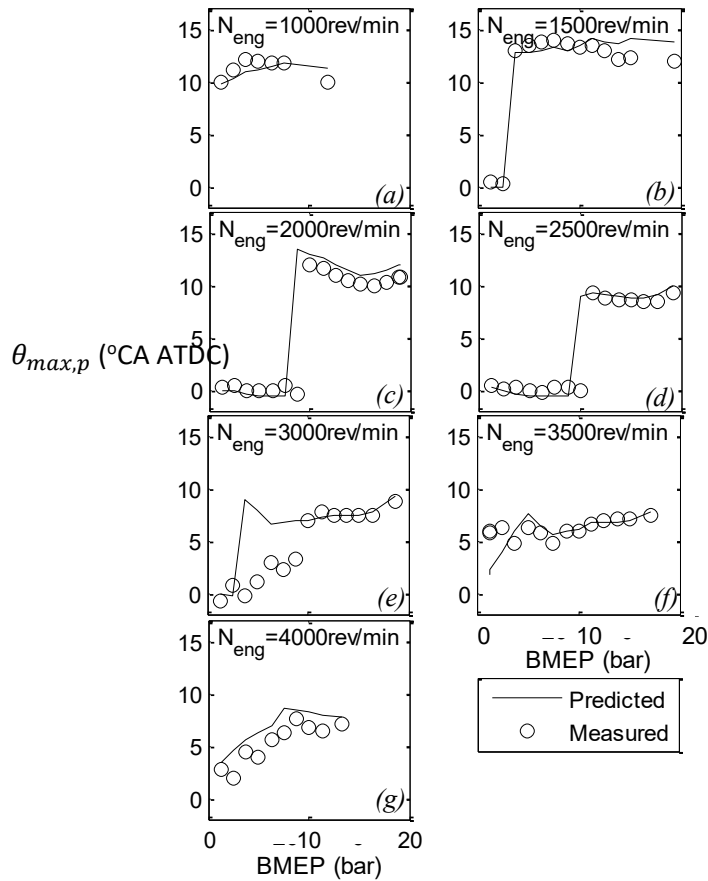


Figure 10: Measured and predicted angle of peak cylinder pressure grouped by operating speeds

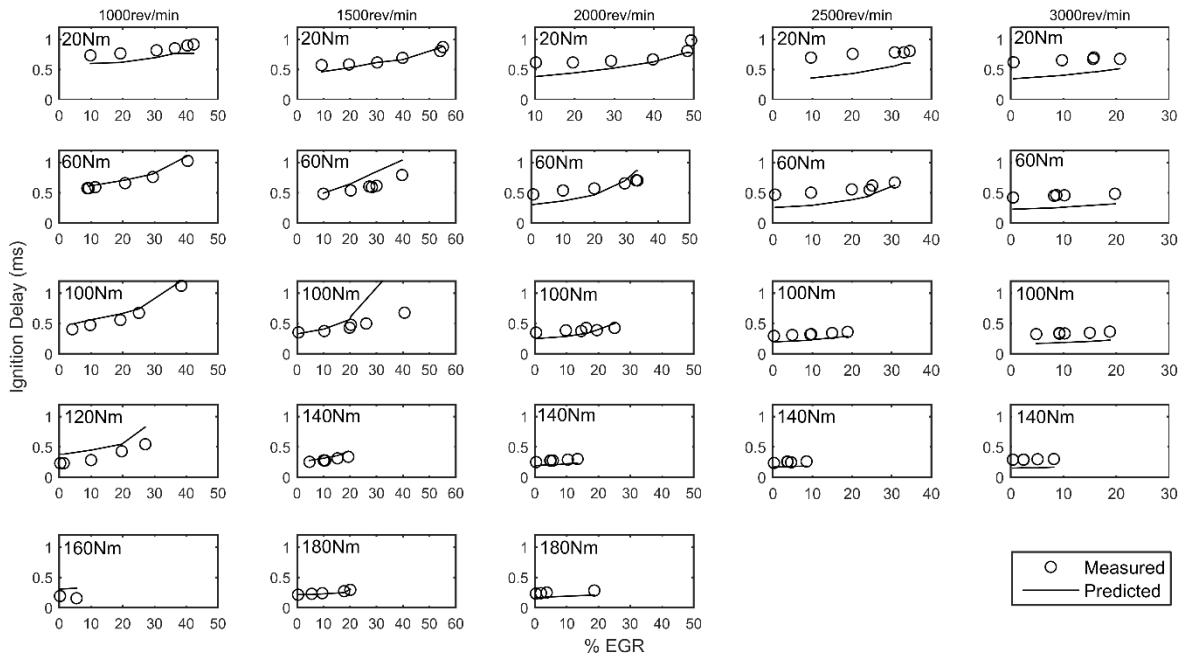
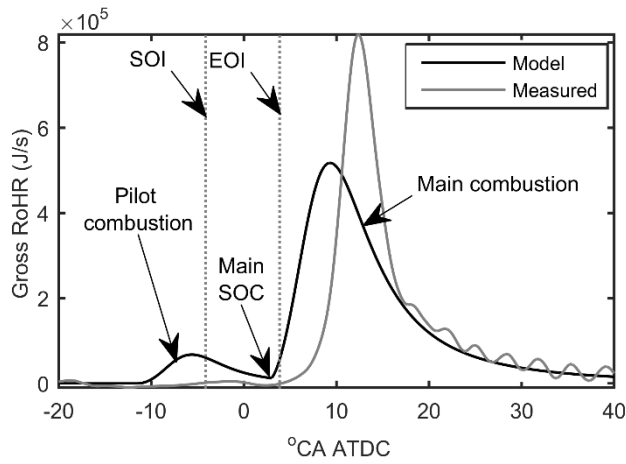


Figure 11: Measured and predicted main injection ignition delay grouped by operating speeds and load for varying EGR rates

1

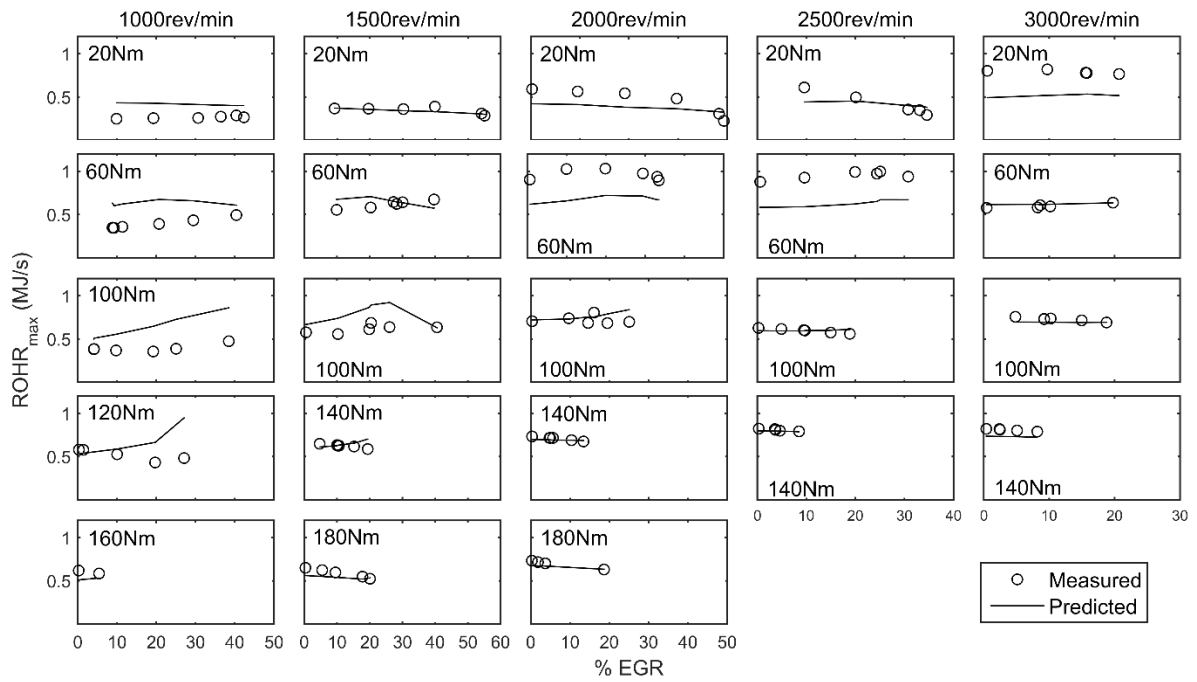


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3

**Figure 12: Example of pilot over-prediction and subsequent under-prediction of ignition delay and peak heat release rate (Engine Speed: 3000rev/min, Engine Load: 20Nm, EGR rate: 10%)**

4



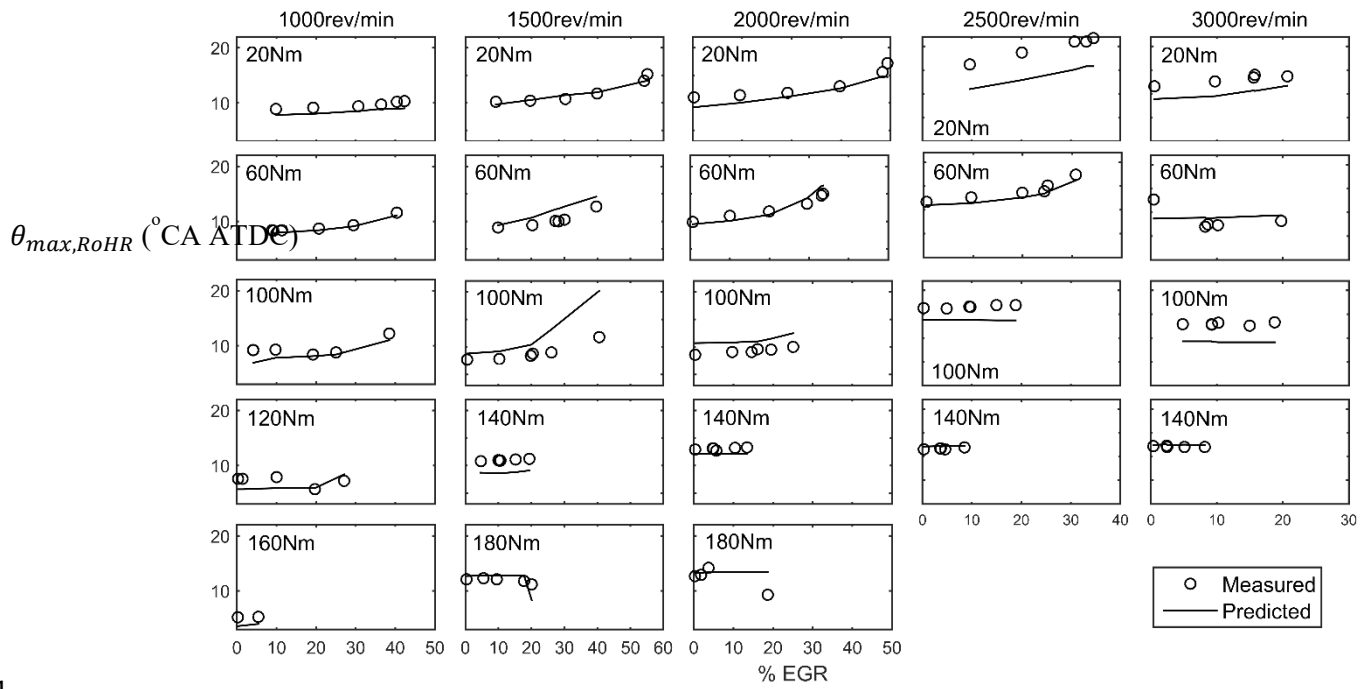
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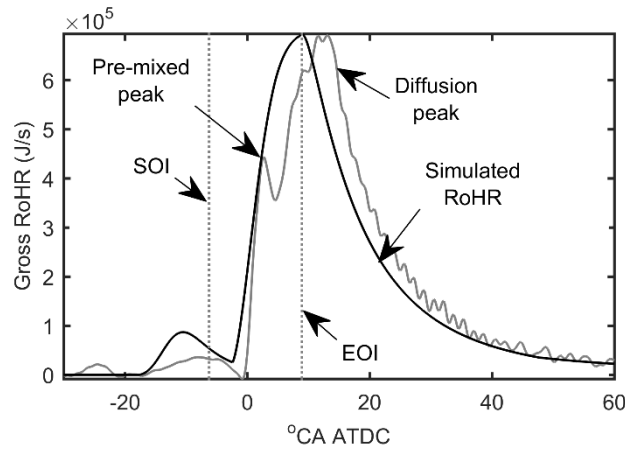
**Figure 13: Measured and predicted peak heat release rate grouped by operating speeds and load for varying EGR rates**

7

8



1  
2 **Figure 14: Measured and predicted angle of peak heat release rate grouped by operating speeds and load**  
3 **for varying EGR rates**  
4



5  
6 **Figure 15: Illustration of the diffusion model over-prediction due to ignoring transport time between the**  
7 **injector nozzle and flame front (Engine Speed: 3000rev/min, Engine Load: 100Nm, EGR rate: 20%)**  
8