Preprint Cambridge Centre for Computational Chemical Engineering ISSN 1473 – 4273

# Identifying optimal operating points in terms of engineering constraints and regulated emissions in modern diesel engines

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released: 1 January 2011

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Preprint No. 118

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*Keywords:* Diesel, Engine, Optimisation, Modelling, Emissions, Combustion

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**Abstract**

In recent decades, ”physics-based” gas-dynamics simulation tools have been employed to reduce development timescales of IC engines by enabling engineers to carry out parametric examinations and optimisation of alternative engine geometry and operating strategy configurations using desktop PCs. However to date, these models have proved inadequate for optimisation of in-cylinder combustion and emissions characteristics thus extending development timescales through additional experimental development efforts.

This research paper describes how a Stochastic Reactor Model (SRM) with reduced chemistry can be employed to successfully determine in-cylinder pressure, heat release and emissions trends from a diesel fuelled engine operated in compression ignition direct injection mode using computations which are completed in 147 seconds per cycle. The model was successfully validated against 46 steady state operating points in terms of in-cylinder pressure and exhaust gas emissions over a three dimensional matrix comprising ranges of EGR, boost pressure and injection timing. The resulting model was then employed to examine the local in-cylinder temperatures and equivalence ratios and to highlight the main sources of excessive exhaust gas emissions.

With a view of identifying the optimal operating strategy, a parametric sweep comprised of 968 computations were then completed, the results of which were narrowed based on satisfying stable operating limits (i.e. peak pressure, knocking combustion). Excessive exhaust gas emissions were identified to highlight the most suitable regime for minimal emissions. Finally, the potential of this technology is examined by discussing aspects of engine development process which can be accelerated using the tool.

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# 1 Introduction

The adoption of physics-based virtual engineering tools has contributed significantly to the advancement of the modern diesel engine by reducing development timescales and cost by offering engineers additional insight into complex interacting processes, facilitating design of experiments, engineering optimisation, and most importantly enabling highly specialised expertise and analysis to be adopted by its users [16].

In recent years, Stochastic Reactor Models (SRM) have gained an increasing attention from the academic and industrial IC engine development community as they offer the ability to simulate combustion and exhaust gas emissions [2–7, 9–13, 15]. These include partiulate size distributions [13] from multiple fuel sources [2, 3, 10, 11] and are completed in amenable timescales compared to 3D CFD [**?** ], thus enabling their implementation into 1D engine cycle simulation tools [5, 6].

This paper describes the validation of a SRM simulator for diesel combustion using a reduced chemical kinetic fuel oxidation and emissions formation model [14]. To demonstrate the robustness of the computational model, resulting simulations are presented and compared with 46 experimentally derived operating points from a 3D test matrix comprised of ranges of boost pressure, exhaust gas recirculation (EGR) and injection timing. The validated model is then employed at constant EGR to characterise the impact of injection timing and boost pressure and to gain further insight into the experiments by examining the key combustion characteristics which dominate within each regime. For each regime, results are examined in terms of pressure profiles, the local mixture compositions (in terms of local equivalence ratio and temperature) and how these impact on regulated exhaust gas emissions of CO, uHCs, $NO_x$ and PM.

Finally, an optimisation of the operating point is carried out, firstly with respect to identifying those regimes in which the engine is operated safely - that is those which satisfy a peak in-cylinder pressure limit, avoiding knock etc. The final optimisation identifies those regimes in which excessive emissions are expected to then identify a safe, low emission operating condition.

The applications of the simulator to the engine development process are discussed in detail. The areas of application are examined in terms of where such a tool can contribute, i.e. in fundamental engine research and development, advanced engineering and practical development stages of the engine development process.

# 2 Experiments

Tests were carried out on a single cylinder engine based on a modified Perkins 1000 series engine fitted with a high pressure common rail fuel injection system. Specifications were as follows and are presented in Table 1, the engine was a 1 litre single with 4 valve cylinder head, central vertical injector and Ganser Hydromag common rail FIE with Cooled EGR system. The testbed had a boosted and temperature-conditioned air supply with the ability to control back pressure to simulate multi-cylinder engine during exhaust phase. Emissions were measured with automated data capture and test bed control at 0.5 deg

increments. Nominal 500ppm sulphur European on highway diesel fuel was used.

The common rail system was chosen because of its flexibility and pressure capability of up to 160MPa. The system could accommodate pilot injection, multiple injections, and a degree of initial injection rate changes via injector hardware changes. Injection pressure was also hydraulically independent of the engine speed and load conditions. The flexibility of this equipment weighed heavily in the choice of FIE for a combustion research engine.

The EGR system was routed from downstream of the exhaust plenum, via a control valve, through a cooler to before the intake air heater/cooler to give complete independent control over both EGR and manifold air temperature.

**Table 1:** *Engine details.*

| | |
|---|---|
| Stroke [mm] | 127 |
| Bore [mm] | 100 |
| Compression Ratio [ - ] | 17.5 |
| Valves | 4 |
| Injection System | Common rail |

## 2.1 Operating Point

To simplify the overall test matrix, tests were carried out at fixed engine speed of 1500rpm and for a fixed injected fuel mass of 63mg. A total of 46 combinations of manifold pressure, injection timing and EGR mass fraction were tested, these are summarised in Table 2 and are presented in three dimensions in Figure 1.

**Table 2:** *Operating point.*

| | |
|---|---|
| Total number of data points | 46 |
| Engine speed [rpm] | 1500 |
| Total injected fuel/cycle [mg] | 63.0 |
| Manifold pressure [kPa] | 10 to 110 |
| Injection timing [degrees CAD aTDC] | -10 to 10 |
| Injection duration [CAD] | 10 |
| EGR mass [fr.] | 0 to 0.5 |

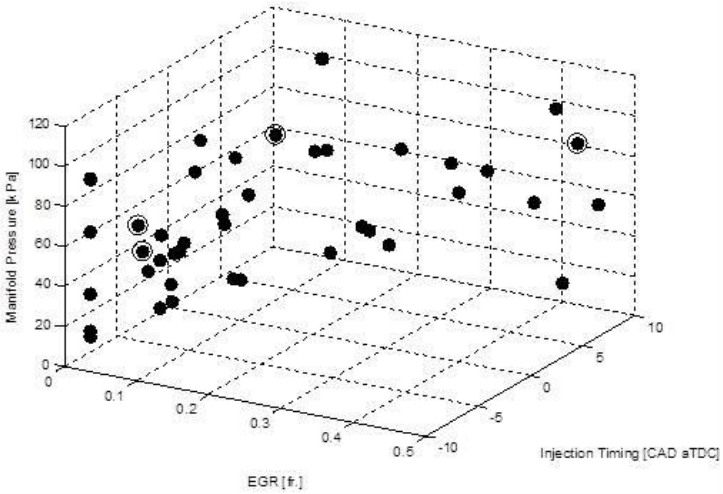



**Figure 1:** *Experimental test points.*

## 2.2 Modelling Approach

### In-cylinder combustion modelling

The Probability Density Function (PDF)-based Stochastic Reactor Model (SRM), an in-cylinder engine combustion simulator (the SRM suite) was adopted for this study [1]. This tool was employed to solve detailed chemical kinetics (crucial for simulating advanced combustion modes) and accounts for inhomogeneities in composition and temperature arising from direct injection, convective heat loss and turbulent micro-mixing. The SRM suite, coupled with a 1D engine cycle software tools, are capable of simulating the combustion and emissions during closed volume period of the cycle (combustion, TDC and negative valve overlap). Furthermore, heat release profiles and in particular the associated emissions (CO, uHCs etc.) can be predicted more accurately than if using the more conventional approaches of the standard homogenous and multi-zone reactor models [1–15].

In this study, SRM suite was applied according to Table 3 and employed to simulate the closed volume portion of the engine cycle, i.e. from IVC to EVO.

**Table 3:** *Engine model details.*

| | |
|---|---|
| Turbulent mixing model | EMST |
| Turbulent mixing time [ms] | 1.7 |
| Heat transfer model | Stochastic |
| Stochastic heat transfer constant [-] | 2000 |
| Wall temperature [K] | 450 |
| Direct injection model | PDF |
| Number of stochastic particles | 100 |

### Fuel oxidation and emissions formation modelling

The diesel surrogate fuel model employed in this study is summarised in Table 4. The level of detail employed by a fuel oxidation and emissions formation model is characterised by its number of reactions and chemical species however an increased number of reactions/species result in an increased computational cost. The original fuel oxidation model has been extended to account for $NO_x$ formation chemistry, however to keep a reduced size and thus retain a fast solution, no chemistry for particulate matter formation processes has been included. This model is considered adequate for diesel fuelled applications as combustion is mainly controlled by fuel injection and turbulent mixing processes, as such the diesel surrogate model employed in this study [14] is considered adequate to properly characterise diesel fuelled combustion applications in reasonable timescales.

One cycle is computed in 147 seconds enabling multiple simulations to be carried out a low computational cost.

**Table 4:** *Chemical model and computational time.*

| Fuel oxidation and emissions formation model | cmcl diesel surrogate with $NO_x$ v1.2 |
|---|---|
| Number of species | 38 |
| Number of reactions | 50 |
| Operating system | 32 Bit Windows Vista |
| Processor | Intel 3GHz single processor CPU |
| Computational time/cycle [s] | 147 |

### Model parameterisation and blind test validation

The model was parameterised by comparing experimental and simulation pressure profiles at the four operating points highlighted with ”rings” in Figure 1. These points were adopted as representative of the range and were considered a typical engine response for the given manifold pressure, injection timing and EGR rate. Parameterisation was carried out on the injection model parameters as well as the turbulent mixing time to achieve the profiles observed in the appendix for these operating points.

In order to formally assess the robustness of any model of this kind, a blind test to examine the ”predictive” performance of the model must be carried out. Hence simulations of the remaining 42 operating points were completed based one set of parameters and by varying only the manifold pressure, injection timing and EGR mass fraction. The computational time for this whole exercise was less than 2 hours in total for the single processor machine outlined in Table 4, however it must be noted that with the adoption of multiple processors as are standard on modern PCs the total time can be reduced proportionally [5].

Resulting simulations were compared with experimental data on the basis of a blind test, the outcome in terms of pressure-crank angle profiles are presented in the Appendix. Generally the model reproduces all the major trends observed in the experiments, in almost all cases differing by less than 5 bar. On an individual cycle basis, it would have been possible to improve each simulation by re-parameterising the model as is required for many

empirical combustion models such as the Wiebe [8]. However, these results are for a single set of model parameters and are considered to be within typical acceptable modelling and experimental uncertainties and satisfactorily mimic the experimental response of the engine to equivalent inputs across a wide range of operating conditions.

The robustness of model is demonstrated when Cycles 38 and 45 are considered. In both cases, the model is inconsistent with the experiment, however these differences are actually associated with mis-reported experimental procedure i.e. the reported experimental injection time is inconsistent with that observed in the experimental pressure profile.

Resulting emissions are presented in Figures A.3 and A.4 in the Appendix. Across the dataset, agreement was considered satisfactory - demonstrating that such a tool can be employed with confidence in the following sections.

# 3 Applications of the model

With the adoption of an increasing portfolio of means to control in-cylinder mixture preparation, combustion and emissions formation, engineers require tools which enable them to (1) simplify the dataset such that the complex interaction of multi-dimensional processes can be examined in manageable sections, and (2) can be employed to facilitate the overall optimisation of the system through intelligent design of experiments. The next section of this research paper examines how the validated model can be applied in these two contexts.

## 3.1 Simplifying and understanding the dataset

Experimental activities have a high capital cost and are limited by the feasibility of fixing interdependent boundary conditions and isolating the impact of a single variable. In addition, physical constraints such as peak pressure, irregular combustion, ”knock” etc. limit these feasible overall operating ranges. This makes insightful comprehensive systematic studies expensive and sometimes unfeasible.

A systematically validated computational model such as that outlined above can be employed to interpolate between experimental data and can be employed to identify and characterise key processes, which may not be able to be visualised using experimental means.

As presented in Figure 1, the experimental data covers some of the composition space of interest. To properly populate the mixture space, 968 simulations were carried out at the points presented in Figure 2.

This exercise was completed on the desktop PC outlined in Table 3 in 84 hours on a single processor. As noted previously, this computational cost can be easily split by running the code simultaneously across multiple processors (i.e. 42 hours on 2 processors, 21 hours on 4 processors etc.) but also through parallelisation of the SRM code itself [5].

**Analysis at 25% EGR mass fraction**

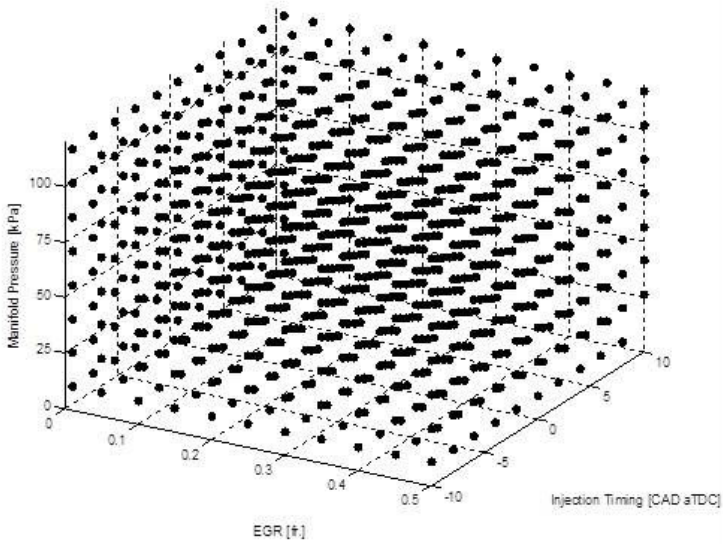



**Figure 2:** *Model resolution points.*

As an example, data obtained with an EGR mass fraction is presented in Figure 3. The following is a summary of the content of this figure

(a) Total equivalence ratio: This is the total mean equivalence ratio within the combustion chamber. Since injected fuel mass is constant, as initial pressure increases, the total air mass is increased thus resulting in a leaner composition.

(b) Timing of 50% mass fraction burned: As injection is delayed, the corresponding onset of ignition and combustion is delayed. In addition, as in-cylinder pressure increases - mean equivalence ratios are leaner resulting in slightly delayed 50% mass burned times.

(c) Maximum rate of pressure rise: This metric has been identified as a means to characterise knocking combustion, earlier injection results in a faster combustion rate and thus knocking combustion.

(d) Peak pressure: Typically the maximum operating peak pressure is a limiting design constraint, in this case, later peak pressures are observed as later injection timings are imposed. At very late ignition timings the peak pressure is due to that of compression not combustion - thus resulting in the horizontal section at 80, 90 and 100 bar.

(e) Peak temperature: As injection is earlier higher peak temperatures are noted due to higher peak pressures, however as EGR is increased lower peak temperatures are noted due to the change in the ratio of specific heat.

(f) Carbon monoxide: This metric scales the level of CO from 0 to 1.0 with the greater concentrations of CO with a ratio of 1.0. Higher carbon monoxide concentrations are reported at high manifold pressures and later ignition timing as combustion is approaching misfire due to lower temperatures at injection and less time for turbulent mixing.

(g) Unburned hydrocarbons: This metric scales the level of unburned hydrocarbons from 0 to 1.0 with the most uHCs with a ratio of 1.0. Similar to that of carbon monoxides but greater emissions are noted at earlier injection timings due to combustion of richer

pockets of gas.

(h) Nitric oxides: This metric scales the level of $NO_x$ from 0 to 1.0 with the most $NO_x$ with a ratio of 1.0. Higher nitric oxides are reported in the same regimes are where higher temperatures and leaner mixtures are observed.

(i) Index of max burned equivalence ratio: This metric scales the level of stratification from 0 to 1.0 with the most stratified cases with a ratio of 1.0. Since the chemical model contained no information for PM formation, this is used as an approximate metric to account for PM tendency. It generally follows the opposite trend to the $NO_x$ formation, i.e. the PM-$NO_x$ trade off.

**Representative cycles**

To further analyse the key processes at these operating points, four representative cycles were identified. These are presented in Figure 4 with the in-cylinder pressure profiles, Figure 4b and equivalence ratio vs. temperature plots. In each equivalence ratio vs. temperature plot, the regimes of increased $NO_x$ (lean and high temperature) and PM (rich and medium temperature) are marked to guide the eye as to the regimes of excessive exhaust gas emissions.

In Figure 4c injection has only occurred in Cycle A and the injected fuel takes one of two paths to combustion (i) it mixes with the reacting zone/burned gases and moves up and along the line of dots making the local equivalence ratio richer, or (ii) when injected the fuel vaporises moving directly toward richer regimes and then it burns and moves to a higher temperature. As shown in Figure 4d at 10 CAD aTDC, this process continues with now many particles having burned at richer equivalence ratios. Cycle D is at a higher initial pressure, thus the local equivalence ratios are slightly leaner than for Cycle A, however higher temperatures are observed resulting in increased $NO_x$. Injection starts at 6 CAD aTDC in Cycles B and C, these both ignite at the moment of injection resulting the the profiles in Figure 4e, Figure 4f and Figure 4g for 15, 20 and 30 CAD aTDC respectively. In these cases, combustion takes place at a lower temperature and over a longer duration resulting in reduced $NO_x$ emissions.

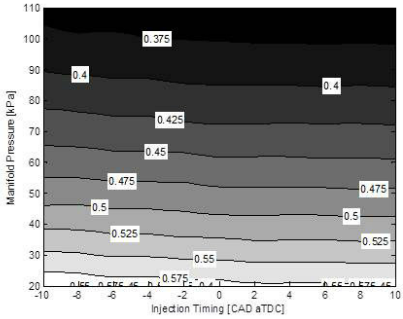
## 3.2 Optimisation of the engine and design of experiments

**Engineering constraints**

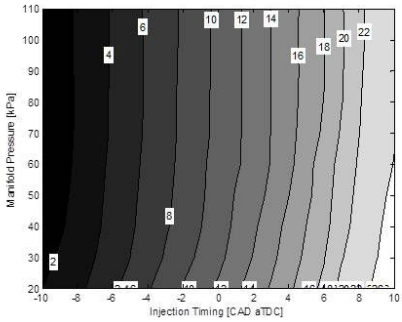
Presented in Table 5 are a list of typical engineering constraints adopted by Caterpillar Inc. which must be satisfied in order for an engine to have a ”safe” extended operating life. The adopted values for constraints such as maximum operating pressure vary depending on specific engine designs so typical values have been employed here.

In this study the temperature in the tailpipe was not simulated, however in the past this has been achieved by implementing srm suite into industry standard cycle simulation toolkits [5].

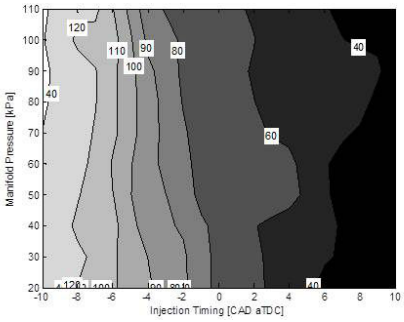
When imposed on the data presented in Figure 3 the overall ”safe” operating regime is limited to the grey to black regimes presented in Figure 3j. This space is mainly reduced by the constraints of maximum peak pressures and knock.



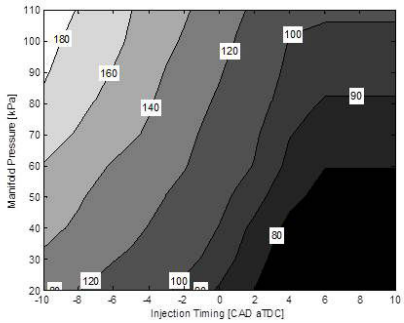

**(a)** *Total equivalence ratio*



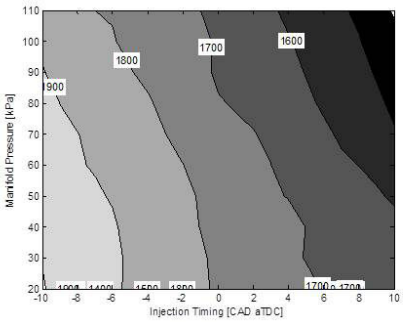

**(b)** *Timing (CAD aTDC) of 50% mass fraction burned*



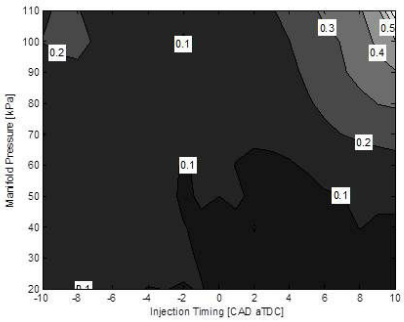

**(c)** *Maximum rate of pressure rise (bar/ms)*



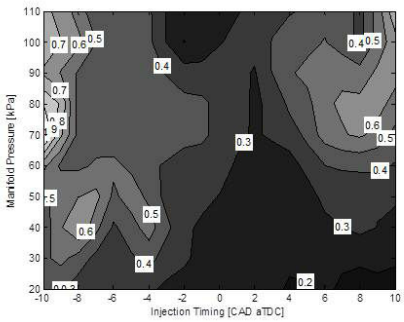

**(d)** *Peak pressure (bar)*



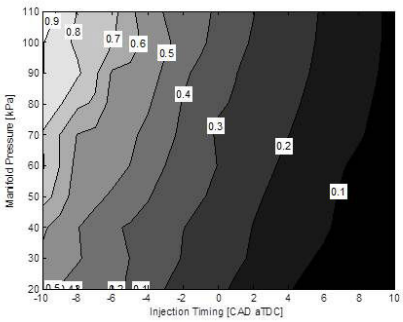

**(e)** *Peak mean temperature (K)*



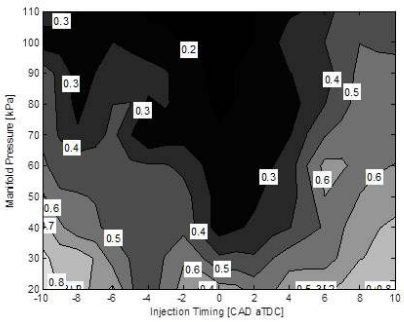

**(f)** *Carbon monoxide emissions*



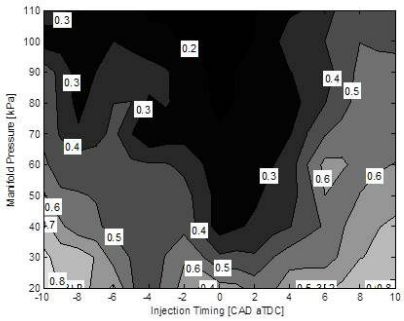

**(g)** *Unburned hydrocarbon emission*




**(h)** *Nitric oxides emissions*

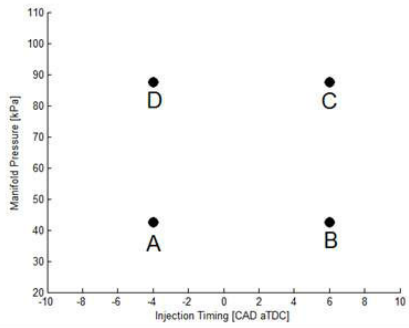



**(i)** *Index of max burned equivalence ratio*

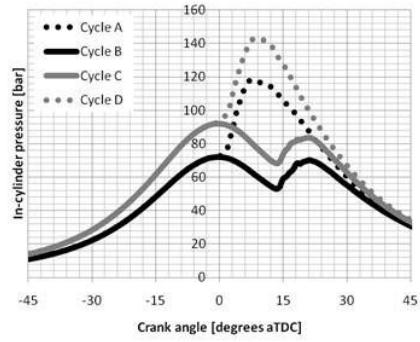



**(j)** *Feasible range at different emission cut offs*

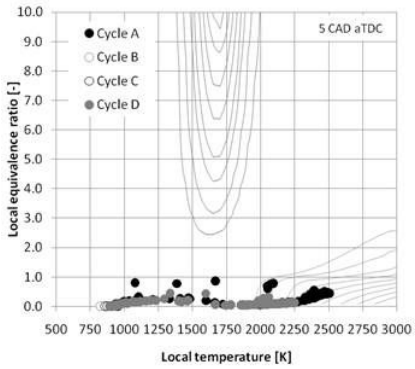
**Figure 3:** *Contour plots obtained at 25% EGR by mass*



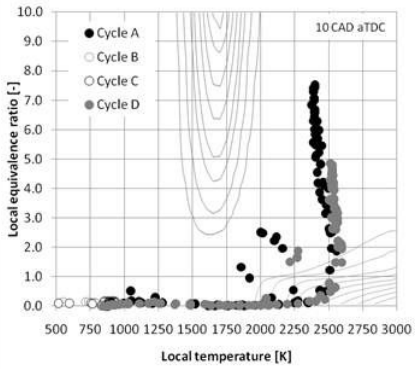

**(a)** *Initial condition*



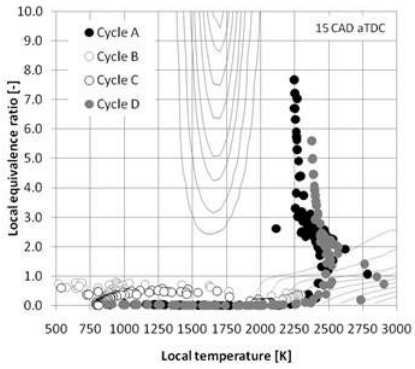

**(b)** *In-cylinder pressure versus crank angle*



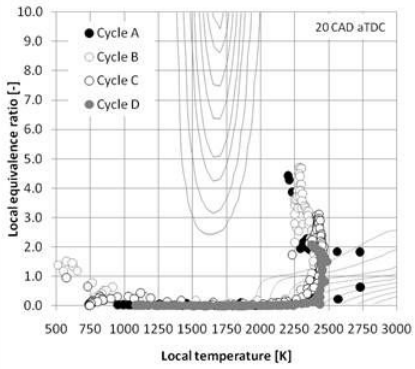

**(c)** *Local equivalence ratio vs. temperature at 5 CAD aTDC)*



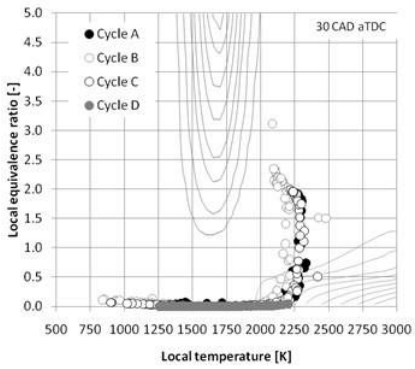

**(d)** *Local equivalence ratio vs. temperature at 10 CAD aTDC*




**(e)** *Local equivalence ratio vs. temperature at 15 CAD aTDC*




**(f)** *Local equivalence ratio vs. temperature at 20 CAD aTDC*




**(g)** *Local equivalence ratio vs. temperature at 30 CAD aTDC*



**Figure 4:** *Representative engine cycles*

**Table 5:** *Engineering constraints.*

| | Characterised by | Imposed constraint |
|---|---|---|
| engine "harshness" | 50% mass fraction burned | $>$ 2 CAD aTDC |
| engine 'knocking and lower-end dynamics | *dp/dt* | $<$ 100 bar/ms |
| Maximum operating pressure / blow-by | Peak cylinder pressure | $<$ 12 MPa |
| Turbo housing and Exhaust manifold durability | Gas Temp at EVO | $<$ 980 K |
| Minimum temperature for Aftertreatment | Temperature in tailpipe | $>$ 495 K |

**Optimisation in terms of emissions**

The objective of employing a fast solution, fuel oxidation and emission formation model was to identify trends, as such the magnitude of particular emissions are important when considering direct trade-offs between emission types such as that reported for PM-$NO_x$. However, for simplicity the emissions were minimised using the following approach.

The remaining area of the diagram is split into emission levels based on Figure 3f, Figure 3g, Figure 3h and Figure 3i. Cuts offs of 0.3 - 1.0 are presented in Figure 3j, the lower the cut off the lower the exhaust gas emissions in that region of the diagram. For a cut-off ratio of 0.5, the area is determined by filtering out all those simulations with emissions greater than 50% of the maximum for any of the emissions species.

Based upon this analysis, the optimal operating point would have a manifold pressure of 60kPa and injection timing of 2 CAD aTDC. This point would be an ideal regime to begin experiments seeking an optima.

**Expanding the analysis to account for the influence of EGR**

The technique outlined above has been carried out across the whole matrix for the full range of EGR mass fractions. Results are presented in Figure 5, highlighting that the optimal operating point is likely to found in with a relatively low EGR composition (0.05 to 0.15), injection timing close to TDC and for a manifold pressure of between 10 and 25kPa.

# 4 Discussion

The key next step is to identify where a tool such as SRM can be employed to exploit its full potential to simulate combustion processes and emissions formation. Presented in

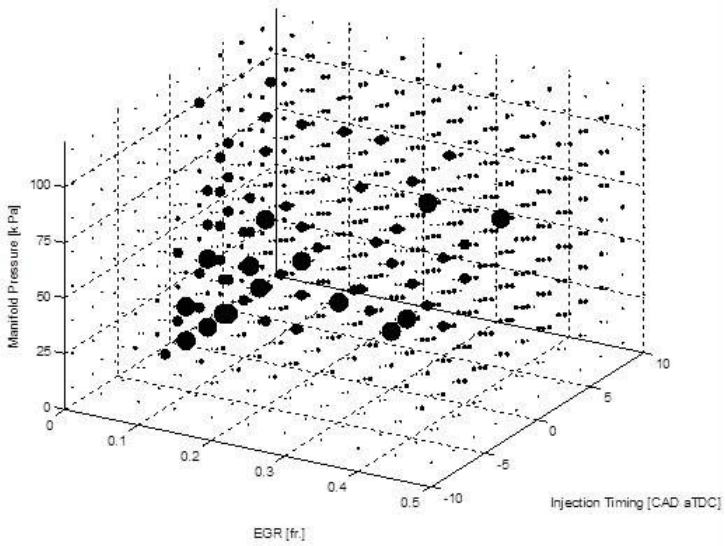



**Figure 5:** *Mixture space showing the most promising operating points - the larger the black mark, the more appropriate in terms of engineering constraints and emissions.*

Figure 6 are a summary of the various stages in the engine development process. In the past, SRM has been employed at Technology Readiness Levels (TRL) 1 to 8, at the Blue Sky level the inclusion of physical modelling has enabled further insight into novel combustion processes such as low temperature combustion [3, 11, 15], adoption of novel fuel blends [2, 10–12, 15], control applications etc. [2]. This research paper has demonstrated how this tool can be employed for diesel engine applications in combination with a 1D cycle simulation code at the TRL levels of 3 to 8 to minimise exhaust gas emissions. These results have particular relevance to a TRL of 7, that is for facilitating engine ”ratings” development. Specifically, by first reducing the feasible operational space, fewer physical trials will be necessary to develop the various engine ratings. Secondly, fast development of engine control and aftertreatment regeneration strategies become feasible as the engine and catalyst system can be accurately modelled as a system.

As an intermediate step to the fully-virtual rating development process, the speed of the current model will enable the performance and emissions engineer to run a model of his engine on a laptop at test cell where they are running the actual engine. This set up will allow the engineer to make decisions on optimising performance calibrations on the fly, and avoid having to shut the engine down to analyse data offline.

When one considers the cost, fuel use and CO2 generated by running 150 engine test cells virtually 24 hours a day, 7 days a week, even a 10% reduction in physical testing could realise millions of dollars in savings. By using tools like SRM, to run engines virtually during ratings development, these savings are entirely possible.

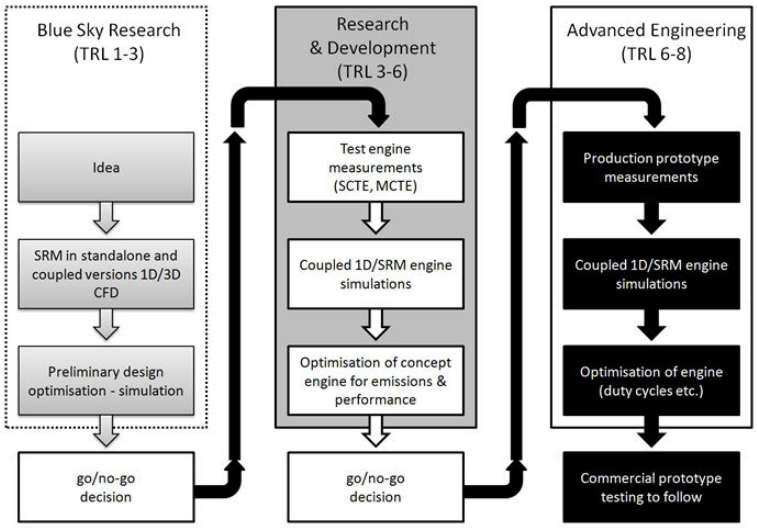



**Figure 6:** *Overall engine development process.*

# 5 Conclusions

In this paper, an advanced combustion model has been employed to simulated diesel combustion. The main findings were;

The outcome of a blind test of the model compared with 46 experimental operating points has demonstrated significant model robustness in terms of pressure profiles and emission trends.

Computational times of less than 3 minutes per cycle simulation on a single node/PC were achieved using a reduced fuel oxidation and emissions formation chemical model.

This enables for parametric studies to be carried out to gain further insight and understanding from limited experimental datasets.

The model can be employed in virtual engine optimisation and intelligent design of experiments.

# A Appendix

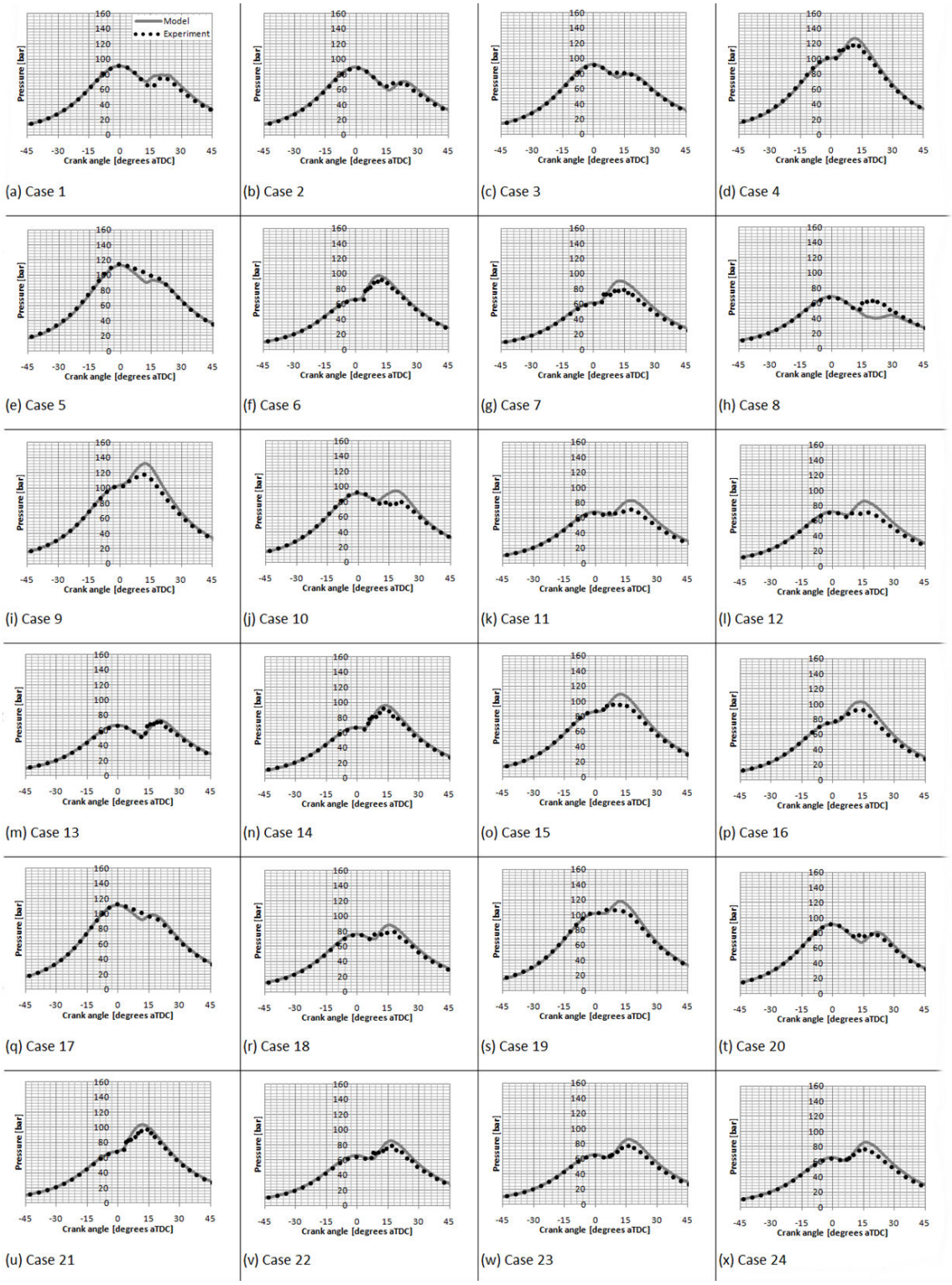



**Figure A.1:** *In-cylinder pressure versus crank angle profiles for model (grey) and experiment (black dots).*

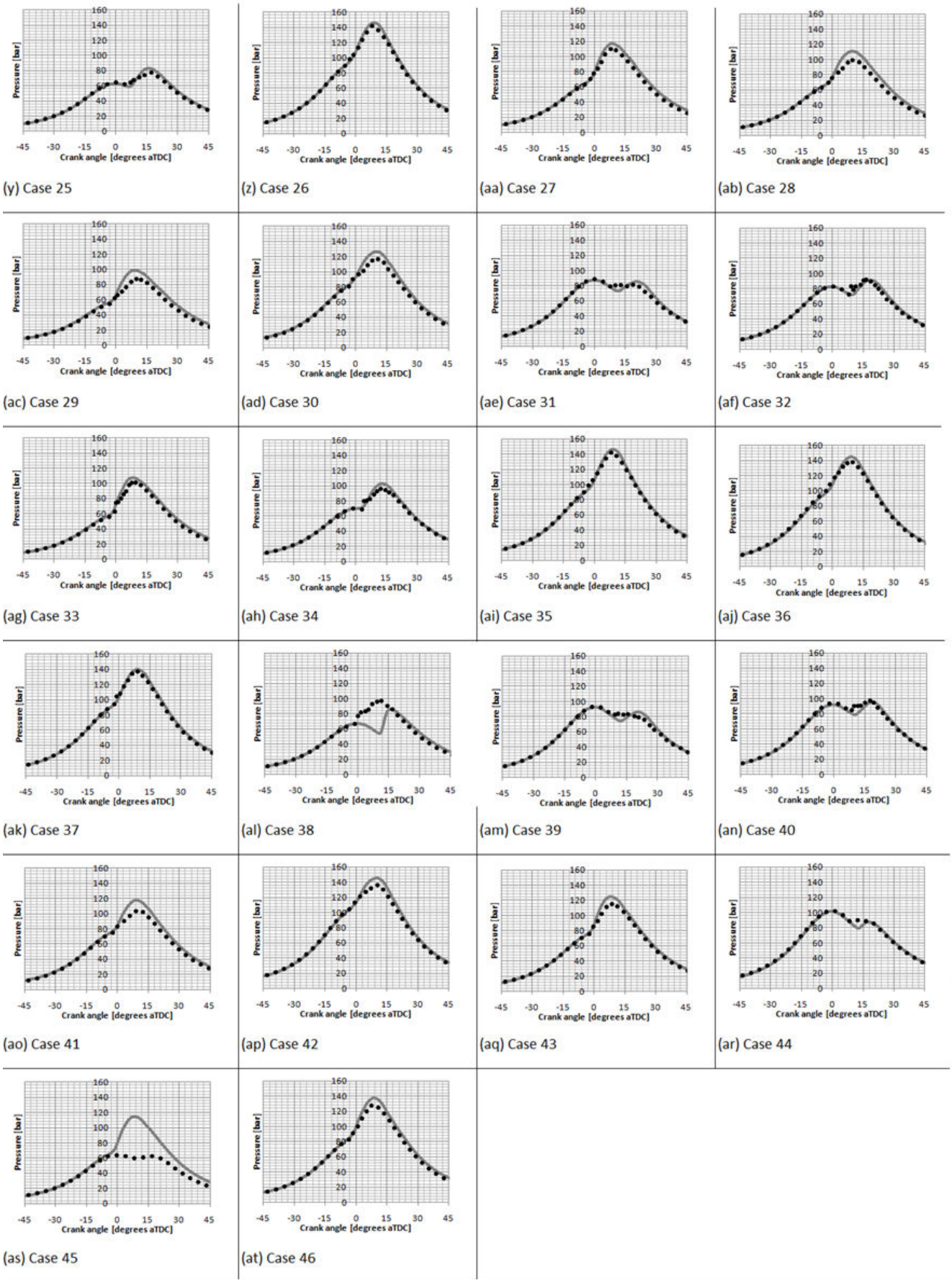



**Figure A.2:** *In-cylinder pressure versus crank angle profiles for model (grey) and experiment (black dots).*

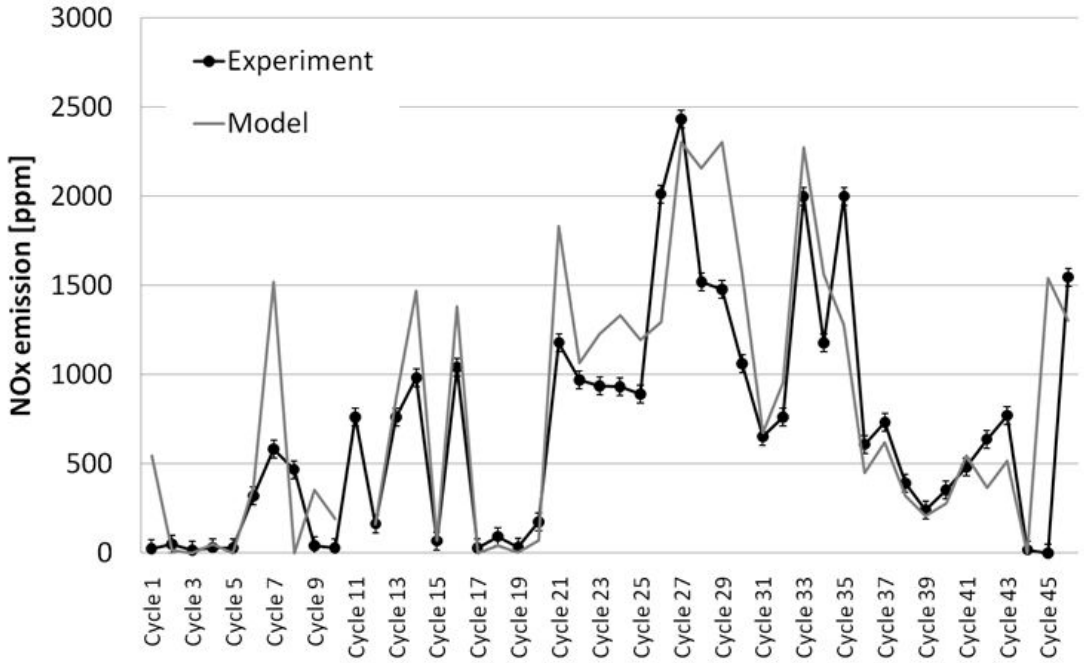



**Figure A.3:** *$NO_x$ exhaust gas emissions for all 46 cases).*

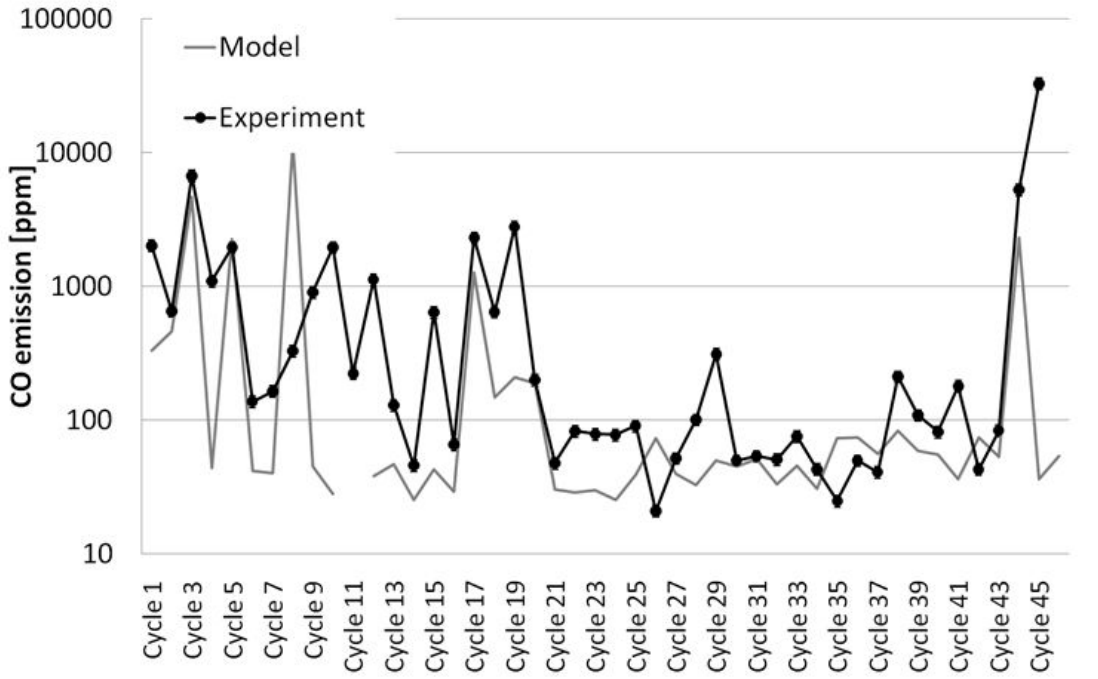



**Figure A.4:** *CO exhaust gas emissions for all 46 cases) and experiment.*

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