Citation for published version:
Bannister, CD & Taylor, J 2014, 'Analysis and empirical modelling to assess and predict the impact of catalyst light-off strategies on the exhaust gas temperatures of spark ignition engines', Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering, vol. 228, no. 14, pp. 1644-1653. https://doi.org/10.1177/0954407013491401

DOI:
10.1177/0954407013491401

Publication date:
2014

Document Version
Peer reviewed version

Analysis and empirical modelling to assess and predict the impact of catalyst light-off strategies on spark ignition engine exhaust gas temperatures

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ABSTRACT

In order to conform to stringent emissions legislation, three-way catalysts have been routinely fitted to gasoline-powered vehicles in order to reduce emissions of carbon monoxide, un-burnt hydrocarbons and oxides of nitrogen. In Europe the majority of all personal car journeys are less than 4 km in length, with the emissions produced in the 1st km accounting for 80% of the total emissions produced in that journey. This is due to the time taken for the catalyst to attain 'light-off' signified by the catalyst reaching a sufficient temperature to allow chemical reactions to occur.

There are a number of methods used to reduce the light-off time such as retarded spark timing, higher idle speeds, artificially loading the engine, secondary air injection and lambda control.

While numerous studies have investigated light-off strategies in isolation, or in limited combinations, this study is the first in open literature to examine all of the above factors simultaneously and to assess how their impact on exhaust gas temperatures varies with distance away from the exhaust ports.

Experimental work was undertaken in order to generate empirical models to predict the effect of gasoline engine catalyst heating strategies on the light-off times of the production three-way catalyst and the exhaust gas temperatures at varying distances along the exhaust system up to, and including, the inlet to the catalyst.

The empirical model demonstrated good accuracy with errors in the temperature predictions, when compared to experimental data, found to be, on average, less than -0.6% at the pre-catalyst location.

KEYWORDS

Empirical modelling, catalyst light-off, gasoline, light-off strategies

NOTATION

ATDC: After Top Dead Center (°CA)

BMEP: Brake Mean Effective Pressure (bar)

BTDC: Before Top Dead Centre (°CA)

CO: Carbon Monoxide

CO_2: Carbon Dioxide

Engine out: Measurement location prior to the catalyst, normally in the exhaust manifold.

HC: Hydrocarbons

NEDC: New European Drive Cycle

NO_X: Oxides of Nitrogen (NO & NO_2)

PM: Particulate Matter

RON: Research Octane Number

RMSE: Root Mean Squared Error

SA: Secondary Air

Tailpipe: Post-catalyst measurement location

TWC: Three-Way Catalyst

INTRODUCTION

In order to conform to stringent emissions legislation, three-way catalysts have been routinely fitted to gasoline-powered vehicles in order to reduce emissions of carbon monoxide, un-burnt hydrocarbons and oxides of nitrogen. For any given journey, the first 150 seconds after engine-start will account for a large proportion of the total emissions produced. A study by Konstantinidis *et al.* [1] found that, for a vehicle equipped with a 2.0 L spark ignition engine and a three-way catalytic converter, the initial 150 seconds of the 800 second-long urban portion of the New European Drive Cycle (NEDC) produced approximately 71% of the carbon monoxide emissions and 55% of the hydrocarbon emissions. This is due to the time taken for the catalyst to attain 'light-off' signified by the catalyst reaching a sufficient temperature to allow chemical reactions to occur.

There are a number of methods used to reduce the light-off time by increasing exhaust gas temperatures such as retarded spark timing, higher engine speeds, artificially loading the engine, secondary air injection and lambda control [2, 3, 4, 5]. Early exhaust valve opening can also be used to increase exhaust gas temperature facilitated via variable valve actuation, but a study by Bohac and Assanis [6] found that although gas temperatures were increased, any benefits attributed to earlier catalyst light off were negated by significant increases in cylinder-out hydrocarbon emissions. Measures taken to reduce light-off times after engine start are often referred to as 'catalyst light-off strategies' or 'catalyst heating strategies'. The essence of all catalyst heating strategies is to increase the temperature of the exhaust gas entering the catalyst and hence increase the catalyst brick temperature more quickly to encourage light-off. It should be noted however, that increased temperature alone is not sufficient to encourage conversion of all exhaust emissions species within a gasoline 3-way catalyst, there must also be a suitable oxidizing agent for the removal of unburnt hydrocarbons and carbon monoxide, and a reducing agent for the removal of NOx [7]. For this reason, for high conversion efficiencies of all three species, the exhaust lambda value must be maintained within a narrow range approximately equal to unity.

A study by Hallgren and Heywood [8] examined the effect of retarded spark timing and secondary air injection on exhaust gas temperature and catalyst hydrocarbon conversion performance on a port fuel injected single cylinder research spark ignition engine. As with other studies, Hallgren and

Heywood found that retarding spark timing by 15°CA increased exhaust gas temperatures significantly (approximately 45% at 1500 rpm, λ=1) resulting in reduced catalyst light-off times. Operating the engine under rich conditions (λ_{engine} = 0.85), in conjunction with secondary air injection, was found to yield the highest exhaust gas temperature entering the catalyst and, as a consequence, the lowest hydrocarbon emissions.

Chan [9] examined how engine control parameters such as idle speed, spark timing and exhaust lambda could be optimized for reduced catalyst light-off times using a Ford MVH 418 spark ignition engine with electronic fuel injection. It was found that exhaust gas temperature could be increased from baseline values by 200°C via retarding the spark timing by 30°CA from the nominal condition. The change in spark timing was found to reduce catalyst light-off times by 86%, with the author stating that further improvements were observed when the cold start idle speed was increased from 1750 to 2000 rpm.

While numerous studies have investigated light-off strategies in isolation, or in limited combinations, this study is novel in that it aims to examine all of the above factors simultaneously, to assess how their impact on exhaust gas temperatures vary with distance away from the exhaust ports and to construct an empirical model which can be used to predict the magnitude of and changes in exhaust gas temperature caused by engine calibration changes. These predictions could have a significant impact on the decision making process during the design and development of new exhaust systems by considering how changes in packaging will affect the exhaust gas temperature at the catalyst entry and the corresponding impact on light-off times.

EXPERIMENTAL METHODS

FACILITIES – Experimental work was conducted using a 215kW AC transient engine dynamometer at the University of Bath allowing steady state testing and transient schedules with modeled gear shifts.

The facility is equipped with two Horiba MEXA 7100 DEGR emissions analyzers for simultaneous pre and post catalyst emission measurements.

The engine used in this study was a VW group 1.8L, turbocharged, port-injected gasoline engine. Further engine details are given in Table 1. The engine was equipped with a production secondary air injection system and three-way catalyst. The production exhaust manifold was removed and replaced with a stainless steel tubular manifold thus removing complications surrounding the thermal mass of the turbocharger and effectively rendering the engine as naturally aspirated as opposed to turbocharged. The fuel used in this study was EN228 compliant, 95 RON forecourt gasoline.

INSTRUMENTATION – The tubular manifold was instrumented with 1mm diameter k-type thermocouples at the entry and exit to each runner, after each runner convergence, at the exit to the manifold and immediately before the exhaust gas enters the catalyst. Approximate thermocouple locations are shown pictorially in Figure 1, with measured distances from the cylinder head given in Table 2. Secondary air flowrate was measured directly using a Bosch HFM5 air mass flow meter fitted in the secondary air circuit.

In addition to the standard engine lambda sensor, a Bosch LSU4 externally-heated wide-band lambda sensor (Lambda 0.7 – infinity) was fitted to the exhaust system before the catalyst entry. Power to this sensor was supplied at least 20 seconds prior to the start of each test to allow it to attain its required operating temperature and generate accurate data from engine start.

The engine was connected to a development ECU allowing changes to calibration parameters to be made via ETAS's INCA software and associated hardware.

Table 1 - Engine Specification Data

Factor	Description
Engine Type	Spark Ignition
Number of Cylinders	4
Engine Displacement (cc)	1781
Cylinder Bore (mm)	81
Cylinder Stroke (mm)	86.4
Compression Ratio	9.5
Fuel Injection System	Motronic ME7.5
Valve Gear	DOHC, 5 valves / cylinder. Variable cam timing
Boost pressure (bar)	0.6
Max Torque (Nm)	225 at 1950-4700 rpm
Max Power (kW)	120 at 5700 rpm

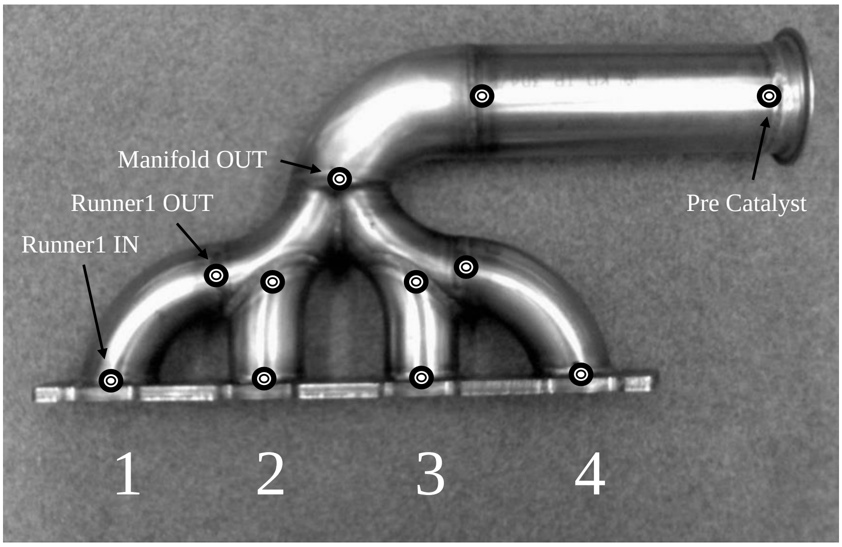


Figure 1 - Tubular manifold thermocouple locations and naming convention

Table 2 - Thermocouple locations and distances from engine cylinder head exit. Where flows converge, the average is taken.

Thermocouple Location	Distance (m)
Runner 1 IN	0.00
Runner 1 OUT	0.12
Manifold OUT	0.49
Pre Catalyst	0.79

APPROACH – In order that other calibration factors, such as cam switching, did not interfere with the light-off investigations, it was decided that variations would be assessed under simplified engine operating conditions. From cold (15 - 20°C), the engine was cranked and allowed to idle for a period of 2 minutes, at which point catalyst heating strategies would be deactivated (via a time-dependent trigger within the strategy) and the engine would be stopped. A maximum test time of 2 minutes was chosen due to the secondary air pump manufacturer's recommendation that, to prevent overheating, the pump should not be operated for more than 2 minutes continuously. Evaluation of catalyst light-off over transient drive cycles was considered, however, within the base-engine calibration, many catalyst-heating strategies were automatically deactivated once the engine speed exceeded a pre-determined value. This would have resulted in the catalyst heating strategies being operational for a far-reduced duration during a transient cycle, thus lessoning their impact.

Within the engine calibration it was possible to define the duration of the catalyst heating procedure (2 minutes) and values for numerous other parameters during that period. The catalyst heating parameters investigated, as well as the range of values, is given in Table 3.

Table 3 - Catalyst heating strategy parameters and ranges

Parameter	Minimum Value	Centre Value	Maximum Value
Idle Speed (rpm)	950	1225	1500
Spark Timing (°BTDC)	-15.0	-7.5	0.0
Engine Lambda (#)	0.78	0.94	1.1
Secondary Air Flow (kg/hr)	0.0	7.5	15.0
BMEP (bar)	0.0	0.5	1.0

The original experimental test conditions were derived using a design of experiments (DoE) approach based on a box-Behnken design [10] incorporating 48 individual test points. Practically however, within the engine control strategy, it was not possible to directly request specific values of lambda and spark timing, instead, multipliers and constants needed to be modified which led to a knock-on effect on the desired parameter. This resulted in a larger than expect number of experimental points as the factors were modified on a trial and error basis to achieve the timing and lambda set points. Although significantly increasing the duration of the experimental programme, these additional test points provided useful data and further populated the design space. Design space coverage will be discussed together with the experimental results.

RESULTS & DISCUSSION

DESIGN SPACE COVERAGE – As has already been mentioned, despite the experimental programme being based upon a box-Behnken DoE design, a large quantity of additional data was collected. Figure 2 shows all collected experimental data points in the stated dimensions, which clearly exceed the original 47 points required for the box-Behnken design.

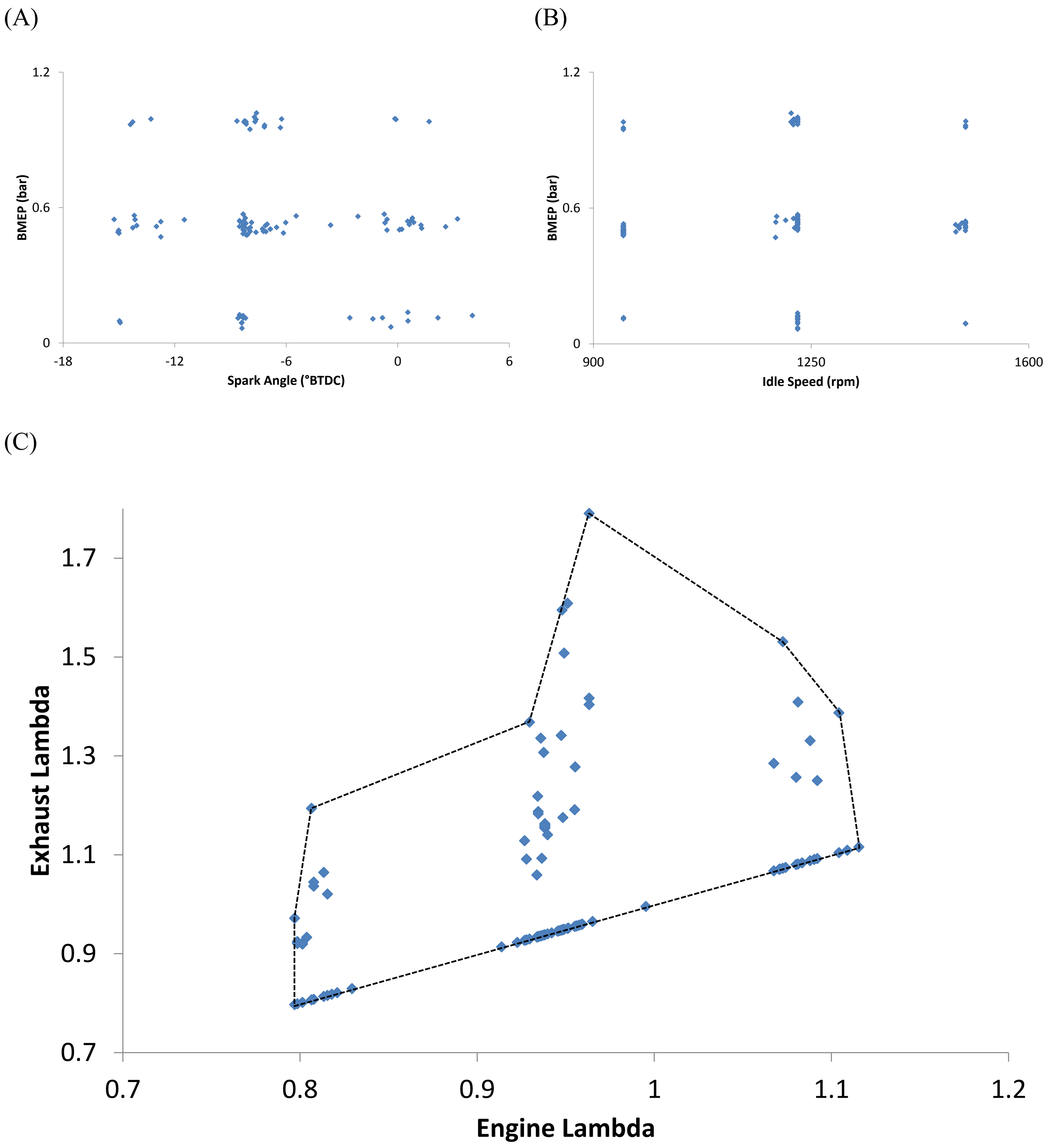


Figure 2 - Experimental design space coverage. (A) BMEP/Spark angle dimension, (B) BMEP/Idle speed dimension and (C) Exhaust Lambda/Engine Lambda dimension.

It should be noted in Figure 2 that, instead of showing secondary air flow directly, the measured additional air flow added to the exhaust stream is included in the measured 'exhaust lambda' value, whereas 'engine lambda' represents the lambda value present within the combustion chamber prior to the addition of secondary air. Examination of Figure 2(C) demonstrates this with a clearly defined boundary where engine lambda is equal to exhaust lambda in the case where no secondary air is added. The region of the plot corresponding to low engine lambda values but exhaust lambda values greater than approximately 1.2 is not populated, as even the addition of 15kg/hr of secondary air is not sufficient to raise the exhaust lambda to higher values.

CATALYST LIGHT-OFF TIMES – A Matlab script was written to align all pre and post catalyst emissions data with the initial engine cranking event so that catalyst light-off times could be calculated at each test point. Light-off was defined as the time at which catalyst conversion efficiency first exceeded 50%. Figure 3 gives an example of the catalyst conversion efficiency for CO, HC and NOx during a test, along with calculated light-off times for each species. If 50% conversion was not achieved within the first 120 seconds of the test (120 seconds being the catalyst heating stage duration), it was deemed that light-off had not occurred for that species under those conditions.

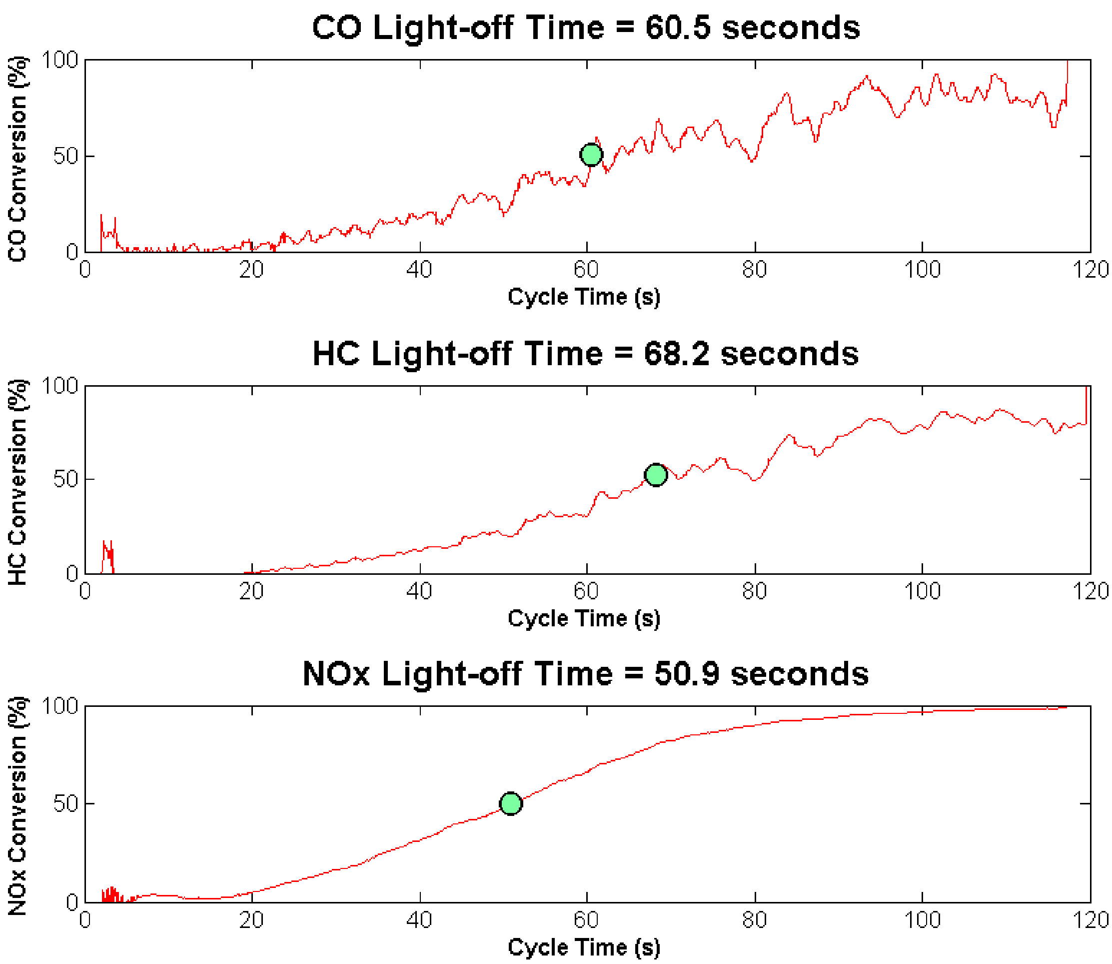
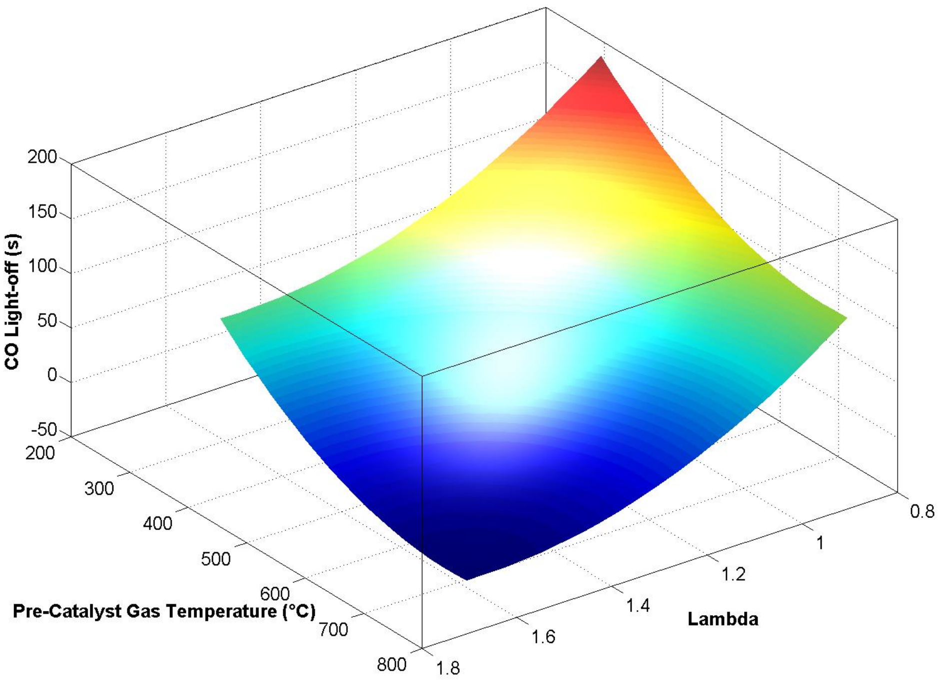


Figure 3 - Example of calculated CO, HC and NOx light-off times. Test condition: 950 RPM, -7.1° BTDC spark angle, 0.5 bar BMEP, engine & exhaust lambda = 1.

The Matlab Model Based Calibration, MBC, toolbox was used to conduct multi-variate analysis of the collected light-off time data. As light-off times were not available at conditions where light-off was not attained, these data were omitted. Figure 4 shows the quadratic response surfaces fit to the experimental data for CO light-off times.

(A)



(B)

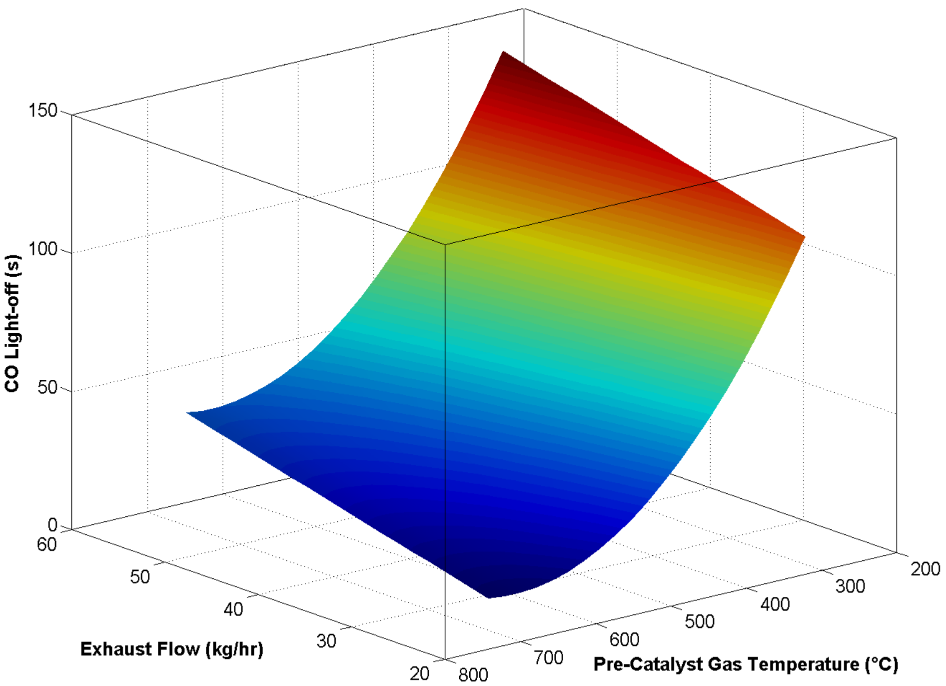


Figure 4 - Quadratic response surfaces for CO light-off times. (A) Gas temperature / exhaust lambda. (B) Gas temperature / exhaust flow rate at lambda = 1. (Model R^2 = 0.74, RMSE = 15.9)

Examining Figure 4, it can be seen that increasing exhaust gas flow rate through the catalyst leads to an increase in light-off times due to a corresponding reduction in gas residence times within the catalyst and the resulting reduction in effective species conversion.

As the oxidation of CO to CO_2 is dependent on the availability of oxygen, it follows that increasing exhaust lambda values lead to a reduction in light-off times. Similarly, under rich conditions (Lambda < 1) light-off times tend towards values greater than 120 seconds implying that there is not sufficient oxygen available for the oxidation of CO. It should be noted that catalyst parameters such as precious metal loading, surface area and aging will have an impact on absolute values of the light-off times, but it would be expected that the trends observed in Figure 4 would remain representative.

Increasing the temperature of the exhaust gas entering the catalyst leads to a significant reduction in light-off time across the lambda and exhaust flow rate range. The gas temperature itself can be increased through variations in the calibration factors outlined in Table 3, and predicting the impact of these factors must be addressed.

EXHAUST GAS TEMPERATURES – The catalyst heating parameters outlined in Table 3 are often employed in order to increase the temperature of the exhaust gas leaving the combustion chamber, or to promote the continuation of exothermic reactions within the exhaust gas stream as it travels through the exhaust system. Figure 5 shows the impact of introducing 15kg/hr of secondary air into an initially slightly rich ($\lambda=0.94$) exhaust stream. In the case where no secondary air is added to the exhaust gas leaving the combustion chamber, clear temperature drops are evident as the gas travels through the manifold and catalyst losing heat to the surroundings.

It can be seen that the addition of the secondary air into the cylinder head, initially leads to a reduction in the gas temperature entering the exhaust manifold as the hot exhaust gasses mix with the cold additional air. Unlike in the initial case, with secondary air added there is no significant temperature drop as the gas travels through the manifold runner as heat is being added to the gas via exothermic oxidation of the excess fuel present in the exhaust stream. Once the gasses reach the catalyst entrance, the temperatures are almost identical with the secondary air case having recovered the 100°C reduction in gas temperature caused by the initial dilution. Clearly this system is not optimized as there was no net benefit of using secondary air on the temperature of the gas entering the catalyst (although there is more oxygen available for reaction with CO and HC demonstrated by the earlier onset of exothermic reactions within the catalyst and corresponding rise in post catalyst temperatures). Decreased engine lambda values, or reduced secondary air flow would likely have resulted in higher gas temperatures entering the catalyst through increased availability of unburned fuel in the exhaust and reduced dilution cooling effects respectively.

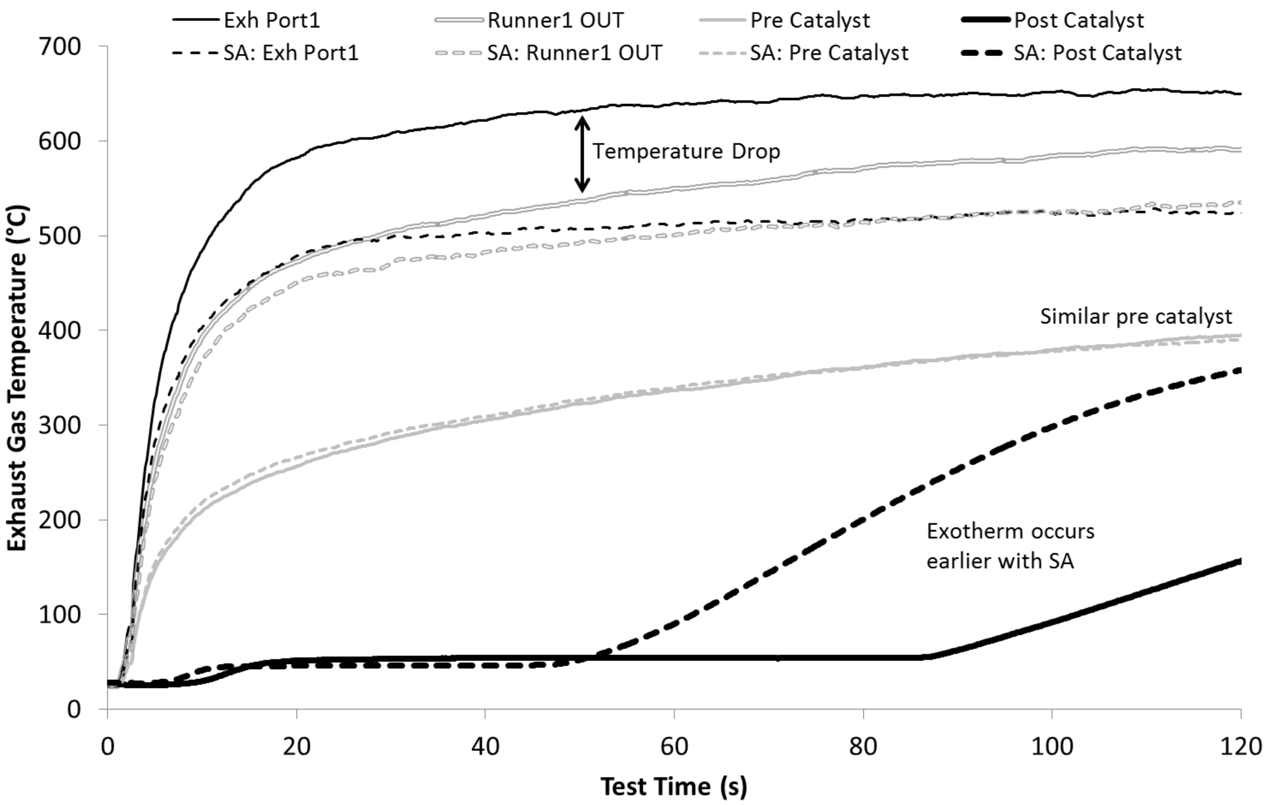


Figure 5 - Effect of secondary (SA) air on gas temperatures within the exhaust system. Dotted lines represent test with 15kg/hr of secondary air added. (Test condition: 950 rpm, -7.5° BTDC spark angle, 0.5 bar BMEP, engine lambda = 0.94)

Figure 5 demonstrates the importance of considering the measurement location when assessing the impact of catalyst heating parameters and, for this reason, the distance travelled by the exhaust gas will be included as an input into the constructed model.

MODEL CONSTRUCTION – Unlike the light-off models discussed earlier which could only include experimental data where light-off was achieved, consideration of exhaust gas temperatures are not subject to this constraint allowing a far larger dataset (108 tests, 4 distances, 432 points in total) to be used to construct the response surfaces. In an attempt to make the model predictions more transferable between different engines and exhaust systems, the model was designed not to predict absolute exhaust gas temperatures, instead predicting a scaling factor which can be applied to a known baseline condition. This approach would allow a calibration engineer to run a single experimental baseline point (or obtain this data through a simulation package such as Ricardo WAVE or GT-Power) which could then be used to predict the impact of calibration changes on these baseline values.

MODEL EVALUATION – As with the light-off time models, MBC was used to generate response surfaces with the output being a baseline scaling factor. A radial basis function with 87 centers was used to fit the surfaces with both a RMSE and press RMSE of approximately 0.04. Figure 6 shows the response surfaces produced within MBC for various combinations of factors. Examination of Figure 6 should be done in conjunction with Figure 2 to illustrate in which regions of the design space extrapolation has occurred and therefore limited confidence in the predictions. Figure 6(A) shows the interactions between engine and exhaust lambda values with maximum scaling factors, and thus increase in gas temperature, occurring under conditions of low engine lambda (0.8) and moderate exhaust lambda (circa 1.4). Further increases in exhaust lambda through continued addition of secondary air leads to a reduction in scaling factor due to dilution effects. Figure 6(B) indicates that idle speed has a very significant impact on exhaust gas temperature demonstrating a 50% increase in scaling factor as the speed increases from 950 rpm to 1500 rpm. Increasing BMEP can be seen to have a small positive effect on gas temperature across the idle speed range. Retarded spark timing, given in Figure 6(C), can be seen to have a very significant impact on gas temperatures resulting in approximately 55% increase at 15°CA ATDC compared to 5°CA BTDC. Increasing BMEP appears to have more impact at advanced spark timings (circa 20% increase as BMEP rises from zero to 1 bar) but, as spark is retarded, this effect is reduced significantly.

Figure 6(D-F) show how the exhaust gas temperature multiplier varies with the measurement location distance along the exhaust system. While there is very little interaction between BMEP and distance, the effect of spark angle and idle speed both demonstrate significant increases with increasing distance. Distance appears to have relatively little effect at low idle speeds and early spark timings, but becomes far more significant at 1500 rpm and retarded spark conditions.

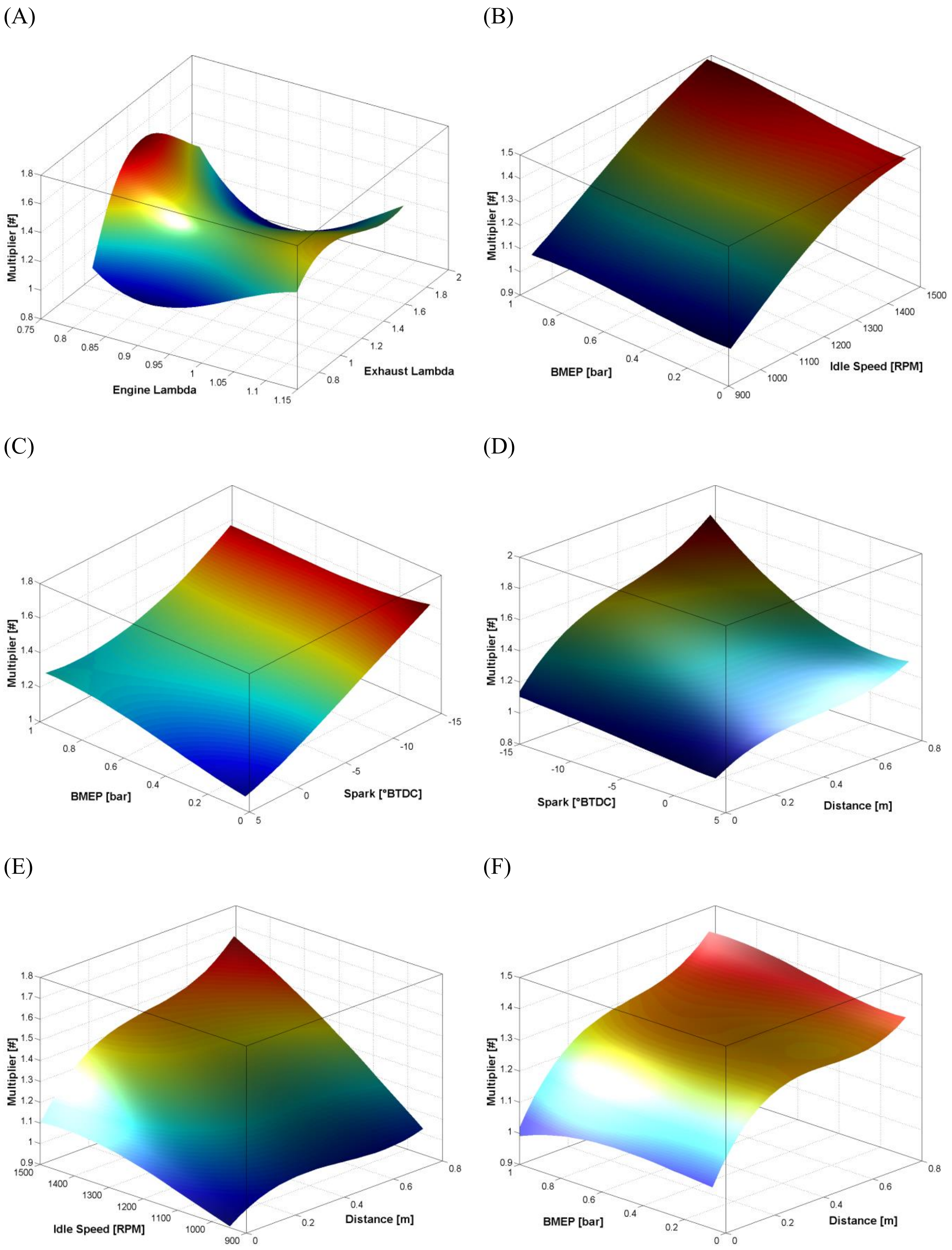


Figure 6 - Exhaust gas temperature multiplier response surfaces. (A) Exhaust Lambda/Engine Lambda, (B) BMEP/Idle speed, (C) BMEP/Spark angle, (D) Spark angle/Distance, (E) Idle speed/Distance & (F) BMEP/Distance.

MODEL VALIDATION – Within MBC the response model can be exported into Simulink and used to make predictions in the time domain. In order to validate the model, experimental conditions (Lambda, spark etc.) not used in the construction of the model itself, were entered into the model to predict the scaling factor which was applied to the baseline experimental data. Predicted results for that condition were then compared to those gathered experimentally.

Figure 7 shows the baseline, predicted results and measured data for a validation test carried out at 950 rpm, 0.5bar BMEP, 0.93 exhaust lambda, 0.93 engine lambda and a spark angle of -15°BTDC. It can be seen that, regardless of measurement location within the exhaust system, the model makes good predictions of exhaust gas temperatures. The prediction error plots show that there is an initial period, immediately following engine start, where the model over-predicts gas temperatures at all locations, however these errors are deceptively large due to the low gas temperatures and, in absolute terms, the magnitude of the errors in °C are relatively small (10°C approx.). After the initial 10 second period following engine cranking, the predictions follow very closely the measured data slightly over-predicting at the runner OUT location (average error = 1.7%, standard deviation = 0.4). At the manifold OUT and pre catalyst locations the model slightly under-predicts the exhaust gas temperature by, on average, -0.8% (S.D. = 0.6) and -0.6% (S.D. = 0.5) respectively.

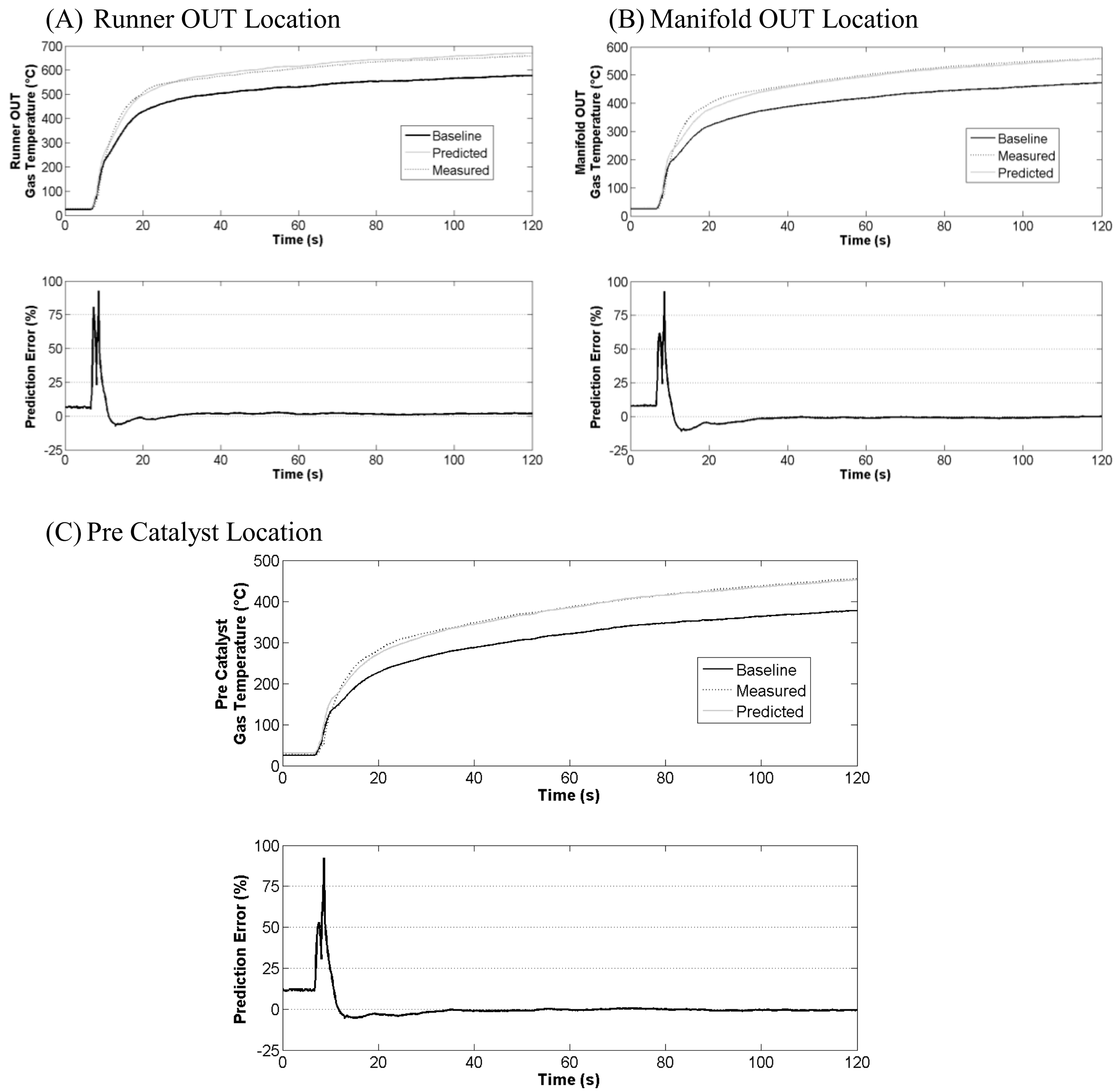


Figure 7 - Multiplyer model validation at three locations within the exhaust system: (A) Runner OUT, (B) Manifold OUT & (C) Pre catalyst locations. Validation test conditions were: 950 rpm, 0.5bar BMEP, 0.93 exhaust lambda, 0.93 engine lambda and a spark angle of -15°BTDC.

CONCLUSIONS

Experimental work was undertaken in order to generate empirical models to predict the effect of gasoline engine catalyst heating strategies on the light-off times of the production three-way catalyst and the exhaust gas temperatures at varying distances along the exhaust system up to, and including, the inlet to the catalyst. Pre-catalyst gas temperature and the exhaust lambda value were found to be the most significant factors on catalyst light-off times.

The empirical model constructed to predict changes in exhaust gas temperatures caused by modifications to the engine lambda, exhaust lambda, idle speed, BMEP and spark timing demonstrated exceptional accuracy when validated using other experimental data not used in the construction of the model itself. Errors in the temperature predictions when compared to experimental data were found to be, on average, less than -0.6% at the pre-catalyst location, but with the error increasing slightly to 1.7% at the Runner OUT location.

Retarding spark timing, by 20°CA was found to result in a 55% increase in gas temperatures while increasing BMEP appeared to have more impact at advanced spark timings (circa 20% increase as BMEP rises from zero to 1 bar) but, as spark is retarded, this effect is reduced significantly. Idle speed was found to have a very significant impact on exhaust gas temperature manifesting in a 50% increase in scaling factor as the speed increases from 950 rpm to 1500 rpm.

The derived empirical model has demonstrated good predictive capability and will provide a useful tool for calibration engineers when assessing the potential impact of calibration changes on catalyst light-off.

ACKNOWLEDGMENTS

The authors would like to thank the RCUK for their financial support through the Academic Fellowship of Dr Bannister. This work was funded by Mahle Powertrain, UK, and undertaken using facilities within the Powertrain and Vehicle Research Centre (PVRC) at the University of Bath, UK.

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