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UTILIZING ALTERNATIVE FUEL IGNITION PROPERTIES TO IMPROVE SI AND CI ENGINE EFFICIENCY

Final Scientific/Technical Report

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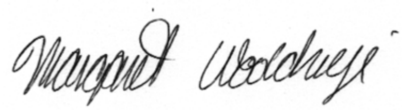

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Utilizing Alternative Fuel Ignition Properties to Improve SI and CI Engine Efficiency

Executive Summary

Experimental and modeling studies were completed to explore leveraging physical and chemical fuel properties for improved thermal efficiency of internal combustion engines. Fundamental studies of the ignition chemistry of ethanol and iso-octane blends and constant volume spray chamber studies of gasoline and diesel sprays supported the core research effort which used several reciprocating engine platforms. Single cylinder spark ignition (SI) engine studies were carried out to characterize the impact of ethanol/gasoline, syngas (H_2 and CO)/gasoline and other oxygenate/gasoline blends on engine performance. The results of the single-cylinder engine experiments and other data from the literature were used to train a GT Power model and to develop a knock criteria based on reaction chemistry. The models were used to interpret the experimental results and project future performance. Studies were also carried out using a state of the art, direct injection (DI) turbocharged multi cylinder engine with piezo-actuated fuel injectors to demonstrate the promising spray and spark timing strategies from single cylinder engine studies on the multi-cylinder engine. Key outcomes and conclusions of the studies were:

1. Efficiency benefits of ethanol and gasoline fuel blends were consistent and substantial (e.g. 5-8% absolute improvement in gross indicated thermal efficiency (GITE)).
2. The best ethanol/gasoline blend (based on maximum thermal efficiency) was determined by the engine hardware and limits based on component protection (e.g. peak in-cylinder pressure or maximum turbocharger inlet temperature) – and not by knock limits. Blends with <50% ethanol delivered significant thermal efficiency gains with conventional SI hardware while maintain good safety integrity to the engine hardware.
3. Other compositions of fuel blends including syngas (H_2 and CO) and other dilution strategies provided significant efficiency gains as well (e.g. 5% absolute improvement in ITE).
4. When the combination of engine and fuel system is not knock limited, multiple fuel injection events maintain thermal efficiency while improving engine-out emissions (e.g. CO, UHC, and particulate number).

Keywords: Spark ignition, compression ignition, ethanol, gasoline, multiple fuel inject events

Comparison of Accomplishments with Project Goals and Objectives

The objective of the project was to demonstrate the combination of fuel selection, fuel injection strategy, and mixture preparation that enables meeting the DOE targets for brake thermal efficiency of greater than 40% for spark-ignited (SI) engines and greater than 50% for compression-ignited (CI) engines. Specifically, the objective of the SI engine research was to identify optimal ethanol/gasoline blend ratios with engine hardware specifics that achieve the DOE VTO goals for engine efficiency and petroleum displacement. The work leveraged the unique and innovative tools and expertise at The University of Michigan to systematically consider the optimal ethanol content of ethanol/gasoline blends, including effects of exhaust gas recirculation, and turbocharging for maximum thermal efficiency, maximum petroleum displacement, and minimal engine-out emissions. The work included physical and computational studies of the pre-ignition/knock properties of ethanol/gasoline blends. The modeling work was used to interrogate and inform the engine studies in terms of identifying the physical and chemical mechanisms affecting the performance of different ethanol/gasoline blend ratios, EGR levels, and boost pressures. The compression ignition work extended the methods of Prabhakar et al. (2015) to demonstrate high efficiency performance of dimethyl ether (DME), propane+DME mixtures and diesel fuel blends over broad speed and load conditions whereas the prior work focused on optimization at a single operating condition. The objectives for each task to support the SI and CI studies are provided below and include comparisons with the actual project results.

Task 1: auto-ignition and spray studies of fuel blends

- *Objectives: to develop ignition and fuel spray correlations that can be used to guide injection and spark timing strategies and can be used in the engine simulations.*
  Several correlations were developed for diesel and gasoline fuel spray development based on new data collected as part of this research project. In addition, elementary reaction chemistry for ethanol and ethanol and gasoline blends were validated in studies supported by additional funding.

Task 2 engine simulations

- *Objectives: to evaluate the impact of knock and flame limits of alternate fuels and combustion strategies on engine efficiency.*
  A new modeling approach was developed to accurately estimate vehicle fuel economy from a sparse set of experimental engine data. In addition, a knock limit model was created to interrogate and interpret the experimental data. Both models were verified with experimental results from this project and from prior studies in the literature.

Task 3: single cylinder engine studies

- *Objectives: to develop spray and spark timing strategies for different fuel compositions and EGR blends that quantify sensitivity to extending knock limits and enabling higher engine efficiencies.*

Two single-cylinder SI engine facilities were used to study a broad range of fuels and engine operating conditions, including different fuel blends with gasoline (e.g. ethanol and syngas), comparison of exhaust gas and air dilution, and boosted air intake pressures. Both engine platforms demonstrated significant improvements in thermal efficiency, engine stability and engine-out emissions using different fueling strategies.

Task 4: multi-cylinder ethanol/gasoline SI studies

- *Objectives: to demonstrate spray and spark timing strategies from single cylinder engine studies on multi-cylinder engine; to assess impact of multiple injection pulses on the knock mitigation and the PM emission for different fuel blends with production and production-intent hardware.*

  The multi-cylinder engine platform used for the study was provided by Bosch, LLC and included the technical support to independently control the fueling strategy. The results of the single-cylinder engine studies of ethanol and gasoline blends were used to select the fuel blends and conditions studied in the multi-cylinder task. The efficiency benefits of ethanol were successfully translated and demonstrated with the production multi-cylinder engine.

Task 5: multi-cylinder DME/propane CI studies

- *Objectives: to demonstrate 50% BTE CI via dual-fueling of DME and propane.*

  The multi-cylinder engine used for this task was a GM 1.9L turbodiesel four cylinder engine, donated by GM. This task was intended to demonstrate 50% peak thermal efficiency at one speed□load condition in the test engine and pursue extension of the operating range and optimization of the combustion strategy, building the prior work by Prabhakar et al. (2013). However, work with the GM test engine did not demonstrate the same efficiency trends with use of DME+propane blends inducted with the intake charge as had been seen in the earlier work with a Euro3 compliant VM Motor 2.5L turbodiesel engine. Through post mortem analyses of the earlier work, it was determined that those experiments under-reported the fuel flow rate of the inducted liquefied gaseous fuel and therefore over-predicted the thermal efficiency gains. Nonetheless, the earlier experiments after re-analysis of that data showed thermal efficiency gains of greater than 5 efficiency percentage points. Such gains were not observed with the GM test engine, and so at the end of Year 1 of the project, this task was sunset as per the Go/No-go decision point in the project plan.

The project milestones and Go/No go metrics are summarized in **Tables 1** and **2**. All Milestones were met on time. The first year Go/No-go metric was not met, and consequently the CI Task 5 was not continued in year 2.

Table 1. Year 1 Milestones and Go/No Go Metric

Milestone	Type	Description	Anticipated Start and Completion Dates	Actual Start and Completion Dates	% complete

Dual-Fuel Studies	Q1 Milestone	Initiate Dual-Fuel Studies	10/1/14 – 1/30/15	10/1/14 – 1/30/15	100
Single-Cylinder Engine Upgrade	Q2 Milestone	Configure and install upgraded single-cylinder engine operation	10/1/14 – 4/30/15	10/1/14 – 4/1/15	100
Multi-Cylinder Engine Upgrade	Q3 Milestone	Configure and install upgraded multi-cylinder engine operation	10/1/14 – 7/30/15	10/1/14 – in progress	100
Fuel Strategies	Q4 Milestone	Develop dual fuel strategies leading to 50% BTE or greater	10/1/14 – 10/30/15	10/1/14 – in progress	100
50% BTE CI Demonstration	Q4 Go/**No Go**	Demonstration of 50% or greater BTE in a multi-cylinder CI engine	10/1/14 – 10/30/15	10/1/14 – 10/30/15	100

Table 2. Year 2 Milestones and Go/No Go Metrics

Milestone	Type	Description	Anticipated Start and Completion Dates	Actual Start and Completion Dates	% complete
Ignition data	Q5 Milestone	Experimental ignition data corresponds with database	10/1/14 – 1/30/16	10/1/14 – 1/30/16	100
Rapid compression faxcility data	Q6 Milestone	Experimental data from rapid compression facility corresponds with database	10/1/14 – 4/30/16	10/1/14 – 4/1/16	100
Knock limits	Q7 Milestone	Demonstration of knock limit extension	10/1/14 – 6/30/17	10/1/14 – 6/30/17	100
40% BTE SI Demonstration	Q8 Milestone	Demonstration of 40% or greater BTE in a multi-cylinder SI engine	10/1/14 – 9/30/17	10/1/14 – 9/30/17	100

Summary of Project Activities

Task 1.1 Auto-Ignition and Spray Studies of Oxygenate/Hydrocarbon Blends

Ignition studies of 100% ethanol and blends ethanol and iso-octane were conducted using the University of Michigan rapid compression facility (RCF) leveraging support from the DOE office of Basic Energy Sciences. Ignition times were measured over a large range of temperatures, pressures and fuel mixtures. Speciation studies were also conducted to provide direct measurements of the fuel reaction pathways. The results are summarized in Barraza-Botet et al. (2016) and Barraza-Botet and Wooldridge (2017). A comparison of the experimental results for ignition delay time and model predictions using the Lawrence Livermore National Laboratory (i.e. Mehl et al. 2011b) are presented in **Figure 1**, and show excellent agreement between the modelling and physical data. Such studies demonstrate high confidence in the elementary reaction chemistry for predicting ignition of ethanol and ethanol and iso-octane blends.

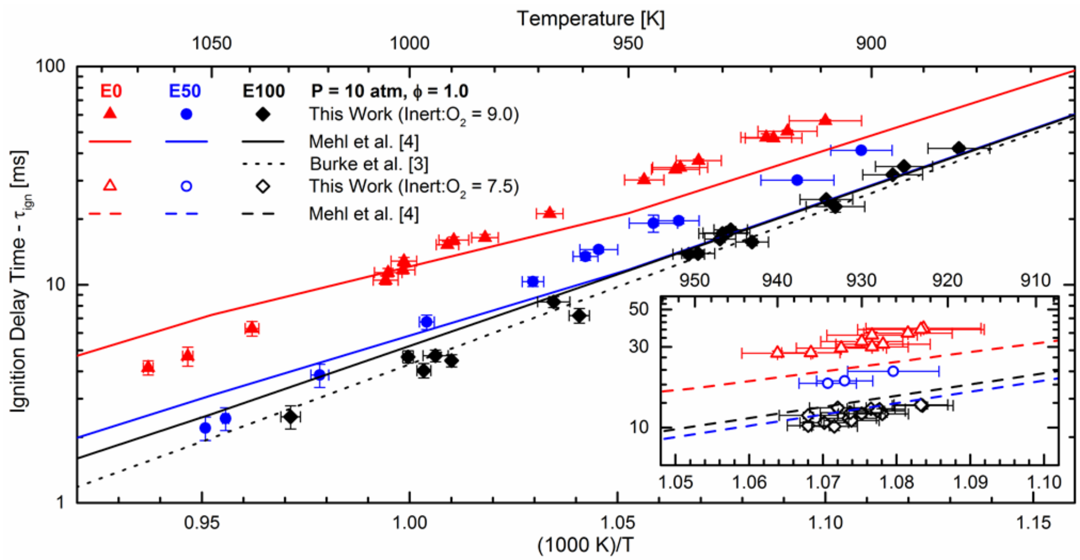


Figure 1. Comparison of experimental results for ignition delay times of ethanol, iso-octane and ethanol/iso-octane blends with model predictions by Mehl et al. 2011b. E0 is 100% iso-octane fuel, E50 is 50% by volume ethanol and 50% iso-octane and E100 is 100% ethanol. Barraza-Botet and Wooldridge, 2017.

The results of a Ford-sponsored research project were also leveraged. In the Ford project, ethanol/indolene fuel blend spray characteristics were characterized in an optically accessible single cylinder engine. The imaging work included spray penetration, spray cone angle and wetted wall length for fuel blends ranging from 0% ethanol/100% indolene to 100% ethanol/0% indolene. Algorithms were developed to quantify air entrainment rates for the different ethanol/indolene blends. This work is summarized in Gutierrez et al. (2015).

Additionally, a recent University of Michigan Ph.D. graduate, Dr. Cesar Barraza-Botet traveled to NREL to work with Dr. Brad Zigler on ignition studies of ethanol/iso-octane blends using the NREL ignition quality tester (IQT) facilities. This effort leveraged the strong foundation of IQT spray studies previously developed by NREL. Dr. Barraza-Botet conducted experiments at overlapping conditions between the UM RCF and the NREL IQT experimental facilities. The two data sets allowed coverage of the largest possible state conditions for validating the autoignition delay behavior of ethanol/iso-octane and ethanol/gasoline blends, as well as comparison of the effects of spray mixing on chemical reaction times. **Figure 2** shows the results of analysis and comparison of the data from the IQT and RCF studies for different ethanol and gasoline blends. The ignition data were used to derive chemical, mixing and evaporation time scale. The results show the temperature dependence is controlled by the chemistry, and as expected the time for mixing and chemistry increase with decreasing temperature and the effects of time for evaporation are small. The data provide valuable insight into the mechanisms controlling reactivity of ethanol and gasoline blends in direct-injection strategies. The journal paper based on this study is currently in review (Barraza-Botet et al. 2017).

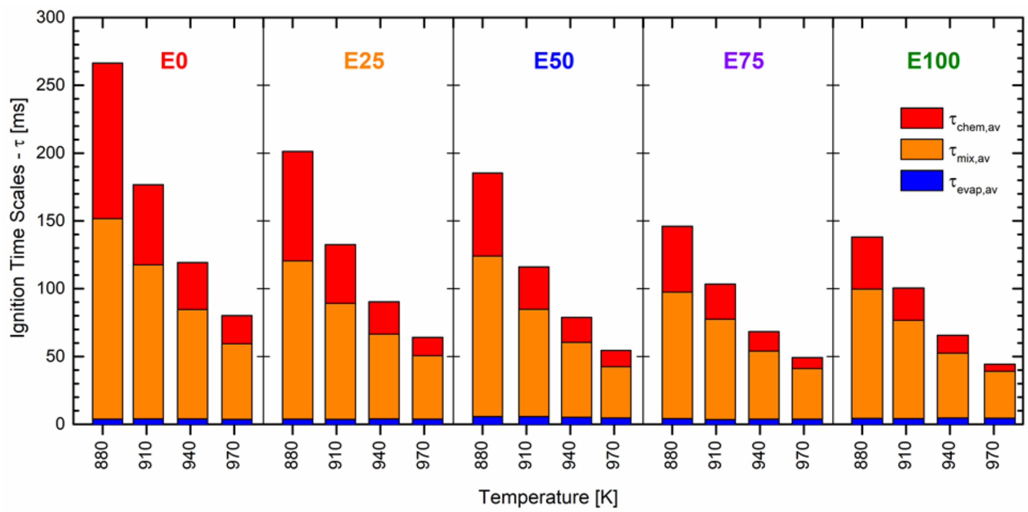


Figure 2. Comparison of time scales at for different blends of ethanol and gasoline as a function of initial charge temperature.

Task 1.2 Simulations of Engine Efficiency Enhancement and Limitations

For this task, a GT Power base engine model was modified to include features particularly important to the thermodynamic studies of the CI and SI engines used in the project. The features included representation of first, arbitrary burn curves, e.g. two stage combustion, and second, the cooling effect of fuel evaporation and its location in the cycle, e.g. port or during compression. Relevant properties of the candidate fuels and fuel blends included heat of combustion, heat of vaporization, specific heats, and where available, auto ignition data. The model predictive performance was validated with experimental engine data from the literature, specifically to calibrate the efficiency related factors such as friction and heat transfer, and observed ignition, flammability and knock limits. The modeling studies considered the effects of ethanol on thermal and volumetric efficiency to complement the experimental studies using the single-cylinder engine. The single-cylinder experimental and modeling results were summarized in Singh et al. (2017a).

Figure 3 shows the results of the investigation of evaporation effects and how they relate to efficiency gains with ethanol and ethanol blends. The data represent experimental results from the Fox single cylinder GTDI engine used in this project which was operated at 1000 RPM over a range of intake pressures from 100 to 150 kPa. CA50 (the crank-angle timing where 50% of heat was released – based on the in-cylinder pressure data) for all points was ~10 degrees after top dead center (ATDC). The ethanol blends were able to operate without knock for all intake pressures while the gasoline point shown is for P_{in} = 100 kPa, which was the only knock-free condition for gasoline. For higher intake air pressures, spark had to be retarded and these results are not shown in **Figure 3**. The curves indicate the GT-Power simulation results which employed a direct injector with the option to take the heat of vaporization from either the walls (with no change in intake temperature) or the intake charge (with significant cooling). Start of injection (SOI) was -240 dATDC corresponding to the engine tests which were all conducted with open valve injection timing.

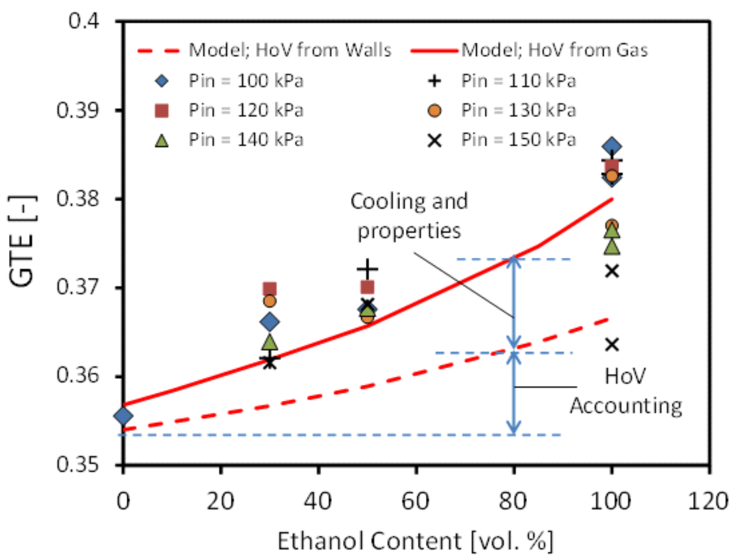


Figure 3. Comparison of GT Power simulation results and experimental measurements of gross efficiency as a function of ethanol content in the gasoline fuel blend. The experimental data (symbols) are from the single-cylinder Fox GTDI engine for various intake pressures. The GT Power results are simulations with all vaporization heat from the walls or with all vaporization heat from the gas.

The two main effects of ethanol fuel are seen in **Figure 3**. The first is simple heat of vaporization (HoV) accounting and is apparent for the case with all heat of vaporization coming from the walls. Since the incoming fuel energy is computed for the liquid fuel, and the heat released is from the vapor state there is a net benefit for the ethanol fuel. For pure ethanol this is about 3.5% efficiency gain on a relative basis. The other effect from ethanol arises from charge cooling and burned gas temperature reduction which will improve gas properties, as well as reduce the amount of dissociation. This is an additional 3.5% for pure ethanol with a total gain of 7%. Similar calculations were carried out with cylinder heat transfer set to zero and the results were almost identical suggesting that any heat transfer changes are small and do not contribute significantly to the efficiency gain with ethanol fuel. Overall the model agrees with the data well. Almost all of the HoV appears to come from the gas. However, for the highest intake pressure (noted by the x symbols in **Figure 3**) and at the highest ethanol levels (E100), there is a significant fall off in efficiency gain - perhaps due to a longer injection event and more impingement on the chamber walls.

Figure 4 shows the results of modeling efforts to identify the impact of fuel ethanol content on knock limited load at 1500 RPM. The experimental data are from a single cylinder study by Stein et al. (2012) at Ford Motor Company, where the authors used a variety of gasoline/ethanol fuel blends and injection strategies, as well as from experiments conducted in the UM Hydra single cylinder engine. The Stein et al. experiments used an 88 RON gasoline and mixed 50% by volume with ethanol, with fuel injected upstream of the intake to eliminate the impact of differing heats of vaporization, while the intake manifold temperature was 52 °C consistent with the RON test conditions. The UM Hydra experiments used an HF0072 research gasoline (HF0072) with an 87 AKI and approximately 30 °C intake manifold temperature. The experiments show a decreasing slope with increasing ethanol content, where the higher ethanol fuel blend enables a higher load for a given combustion phasing (CA50), and a higher load at the latest combustion phasing. The UM experimental data exhibits similar behavior to the Ford results for gasoline with no ethanol addition (E0), with a shift to higher loads consistent with the lower intake manifold temperature and higher octane rating both mitigating the tendency of the engine to knock.

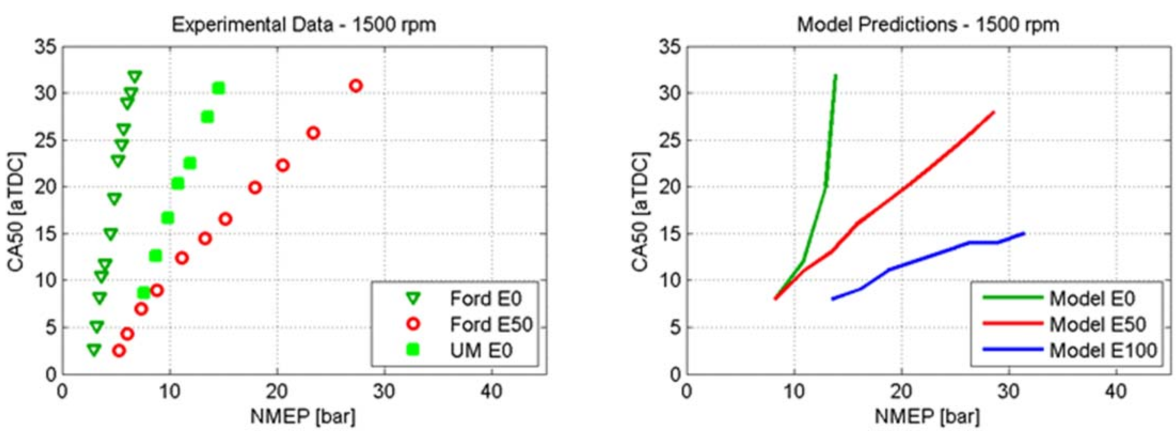


Figure 4. Comparison between experimental and modeled knock limits for gasoline/ethanol fuel blends. The left panel presents experimental data from Stein et al. (2012) and the UM Hydra single-cylinder engine. The right panel presents the variable pressure reactor model results replicating the trend of decreasing slope and higher load limits with increased ethanol content.

A variable pressure reactor model was used to study the experimentally observed behavior. Pressure histories for this model were generated from a GT-Power single cylinder model, which was also used to estimate in cylinder temperature and composition at intake valve closing over the experimental range of intake conditions. The onset of knock was calculated using the gasoline surrogate mechanism of Mehl et al. (2011a, 2011b), which includes an ethanol sub-mechanism and was developed to replicate 87AKI RD-387 research grade gasoline. Knock was defined to occur when the variable pressure reactor ignited (based on fuel mass burned).

Overall the model agrees well with the experiments. The model predictions replicate the experimental trend of higher ethanol fuel blends having lower slopes and achieving higher loads at constant CA50. The E50 results agree well with the experiment in slope and magnitude. While the slope of the pure gasoline results agrees well with the experiments, the predicted NMEP values are all higher than the experiment. This is consistent with the model fuel surrogate having a lower reactivity, particularly in the negative temperature coefficient region, than the experimental fuel, as longer ignition delays would enable higher pressure operation prior to the onset of knock.

The modeling work also included developing a method to estimate fuel economy using limited engine speed and load data. While one of the overarching goals of engine research is to continually improve vehicle fuel economy, evaluating the impact of a change in engine operating efficiency on the resulting fuel economy is a non-trivial task and typically requires drive cycle simulations with experimental data or engine model predictions and a full suite of engine controllers over a wide range of engine speeds and loads. To avoid the cost of collecting such extensive data, some proprietary methods exist to estimate fuel economy from a limited set of engine operating conditions.

The method developed here demonstrates the use of Voronoi partitions to cluster and quantize the fuel consumed along a complex trajectory in speed and load to generate fuel consumption estimates based on limited simulation or experimental results. Detailed vehicle drive cycle simulations were conducted for the FTP, HWY, and US06 cycles using vehicle configurations corresponding to a passenger sedan, crossover, and pickup truck. Several engine maps representing naturally aspirated and downsized turbocharged designs with varying efficiency were considered for each vehicle configuration. The predicted speed and torque visitation points were then used to select a small set of Voronoi anchor points and determine weighting factors to estimate vehicle fuel economy.

Predictions with the estimation method replicated detailed drive cycle results within 0.5 MPG under most configurations tested, using the engine performance at as few as 10 anchor points as input. The engine operating conditions of greatest impact on vehicle fuel economy were in the mid-speed and mid-load region and corresponded to 5 anchor points capturing > 85% of the vehicle fuel consumption on the FTP and HWY drive cycles. An example of the visitation points and the corresponding automatically selected anchor points is shown in **Figure 5** for the FTP cycle for the MY2015 Ford Escape using the 2.5 L naturally aspirated Dual Cam Phaser engine.

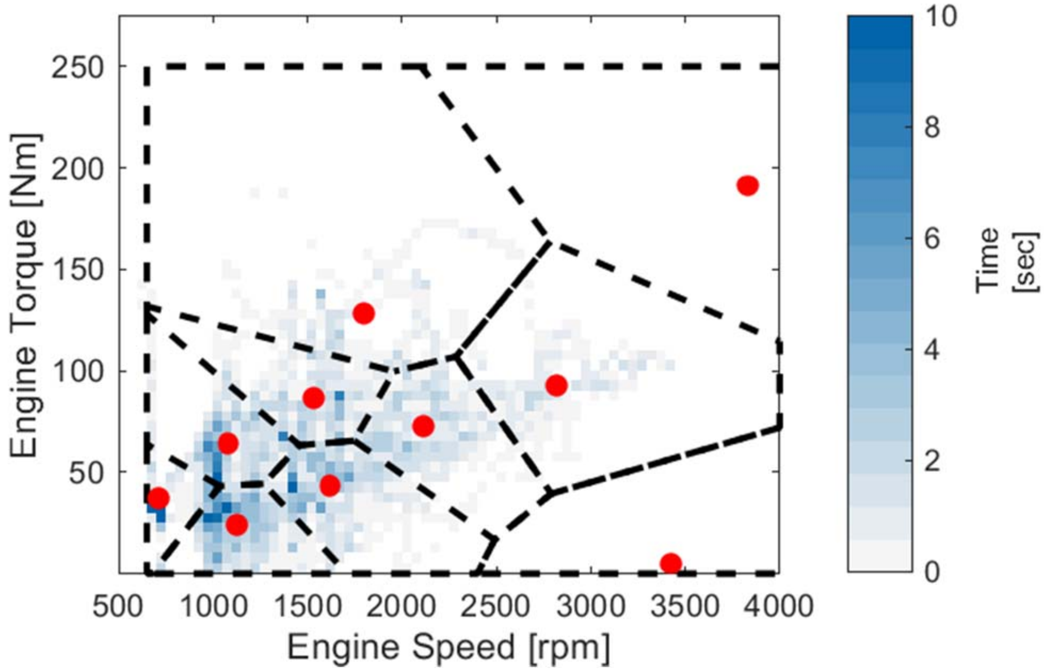


Figure 5. Predicted FTP drive cycle visitation times for the MY2015 Ford Escape using the 2.5 L DCP engine. Voronoi cell anchor point locations (circles) were automatically determined using a weighted Lloyds algorithm.

The predicted fuel economy results are shown in **Table 1** along with the detailed cycle calculation using the full drive cycle simulation. The model results using the automatic engine anchor points are good agreement with the detailed fuel economy estimates. In practice it is desirable to determine a common set of anchor points that can be used during engine development, and that does not depend on the particular combination of engine and transmission choice. For this purpose a set of common anchor points was chosen to represent the major features of the automatically selected points. The final column in Table 1 was generated using these common anchor points. The results are less accurate than the automatically generated cases, but overall acceptable. More details of the analysis can be found in Middleton (2018) recently submitted to the 2018 SAE World Congress.

Table 3. Model predictions of vehicle fuel economy in Miles Per Gallon (MPG). Detailed results are directly from GT-Power simulations using the detailed drive cycle while estimates were made with the visitation point analysis developed in the current work using two different analytical methods.

Vehicle	Engine	Cycle	Detailed Drive Cycle	Automatic Point Estimate	Common Point Estimate
Fusion	2.5L	FTP	26.6	26.8	26.5
		HWY	40.0	40.0	40.8
		US06	26.1	26.5	26.7
	1.6L	FTP	29.7	29.7	29.6
		HWY	43.3	43.3	43.8
		US06	27.3	27.8	28.0
Escape	2.5L	FTP	25.8	25.6	25.8
		HWY	37.1	37.2	37.8
		US06	23.8	24.3	24.5
	1.6L	FTP	28.5	28.3	28.3
		HWY	39.6	39.6	40.3
		US06	24.6	25.2	26.0
F-150	2.5L	FTP	19.8	20.1	20.4
		HWY	26.3	26.2	26.1
		US06	17.7	18.1	18.0
	1.6L	FTP	21.0	21.5	21.9
		HWY	27.7	27.9	28.1
		US06	16.1	18.5	19.9

Task 1.3 Lean-Spray Guided Single-Cylinder Engine Studies to Extend Knock Limits and Mitigate PM/PN

Work for this task focused on preparation of the two complementary test facilities and test engines. In one test cell, a Ricardo Hydra 0.5 L single cylinder engine with a dual overhead cam, pent-roof cylinder head, central mount spark plug and port fuel injection was mounted in a test stand that provided hydraulic dynamometer-based control of engine operation, boosted intake and exhaust flows (up to 3 bar intake boost) and real time engine control. The engine was converted to direct injection spray guided operation by installing a DI fuel injector (HDEV-4) in the engine and moving the spark plug to an off-center location. Bosch LLC provided an engine control unit (ECU) to operate the injector via the test-cell, real-time interface. A Bosch gasoline direct injection (GDI) fuel injector (central mount, spray guided) was acquired for the engine. For the project, a Horiba MEXA 7100DEGR emissions bench was acquired, installed and commissioned to provide gaseous emissions measurement capability for the Hydra single-cylinder engine.

In the second test cell, a production Ford Fox engine was purchased and installed. The production configuration of the engine was as a direct fuel injection turbocharged three-cylinder engine with Bosch LLC fuel injectors. Two of the cylinders were deactivated and the remaining cylinder was instrumented for pressure measurements. Boosted intake air was provided through a centralized compressed air system. Bosch provided a fuel injector control unit as part of the cost share commitment for the project.

Experimental studies using the Hydra and Fox single-cylinder engine facilities were completed. Results of the Hydra engine study were presented at the SAE 2017 World Congress (Han et al. 2017), and results of the Fox engine study were presented at the SAE 2017 Fuels and Lubricants Congress (Singh et al. 2017a). Highlights of the studies are presented here.

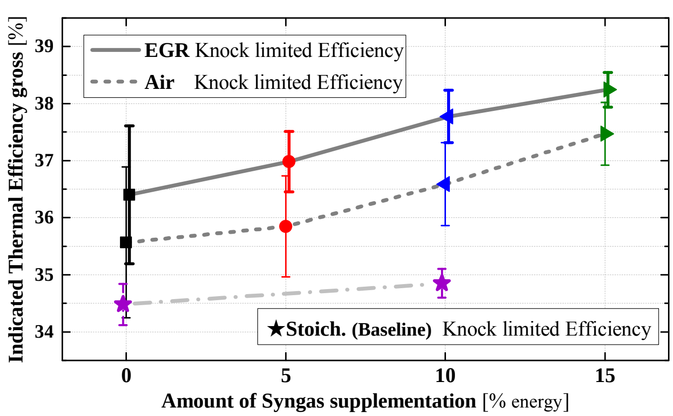
Task 1.3.1 Outcomes from the Single-Cylinder Hydra Engine Facility

Significant progress was made during this project using a port fuel injector (PFI) for understanding sensitivity to knock and robust means of suppressing knock. Comparisons of dilution and fuel reforming showed clear advantages of combining exhaust gas recirculation (EGR) with syngas (simulated reformate) for improving brake thermal efficiency (BTE) and expanding the stable, knock free operating domain.

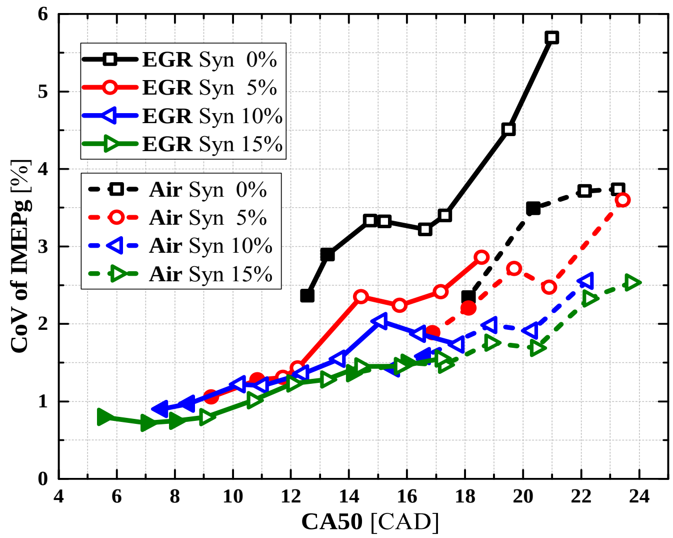
As shown in **Figure 6a**, the overall gross indicated thermal efficiency difference between EGR dilution and air dilution was 1.0 % on average at each level of syngas addition. In addition, the thermal efficiency benefit compared to the baseline of stoichiometric condition was 1.92% and 1.09% under neat gasoline EGR and air dilution conditions, respectively.

The thermal efficiency benefit of varied syngas addition was higher than the dilution benefit in the 0 to 15% syngas addition range. As shown in **Figure 6a**, the gross indicated thermal efficiency consistently increased with increasing syngas amount, and the difference was 1.84% and 1.90% under EGR dilution and air dilution conditions, respectively.

Figure 6b shows the coefficient of variance (CoV) of gross indicated mean effective pressure ($IMEP_g$) for EGR and air dilution. The effect of syngas addition on combustion stability was noticeably higher in both dilution cases. Without syngas addition, the combustion instability with EGR dilution was much higher than with air dilution, but with increasing syngas addition, the stability was improved for EGR dilution. For 15% syngas addition, the CoV of IMEPg with EGR dilution followed the same trend as CoV of IMEPg with air dilution. Thus, the benefits of syngas addition on combustion stability were more pronounced with EGR dilution than with air dilution.



(a)



(b)

Figure 6. Results from the Hydra engine studies of the effects of EGR and air dilution with and without addition of syngas (Syn) (a) gross indicated thermal efficiency of knock-limited conditions and (b) coefficient of variance of IMEPg.

Another area where the Hydra engine experiments yielded significant insights, outlined by Han et al. (2017), is in the area of knock analysis. A spark timing sweep at 1 crank angle degree interval was performed to find the knock limit for each dilution condition while varying the amount of syngas. **Figure 7** shows the spark timing versus combustion phasing (CA50), and the audible knock points are indicated by the filled symbols in the figure. CA50 was clearly decreasing as spark timing advanced, and it is clear that by increasing the syngas ratio, the knock limit approached MBT (between 7 and 10 crank angle degrees) timing.

For fixed spark timing, more knock occurred with increased syngas energy ratio, for instance, the spark timing regions of -26 ~ -28 aTDC for EGR and -16 ~ -17 aTDC for air dilution. However, for fixed CA50, knocking decreased with increased syngas addition. The audible knock method, however, was only able to detect general knock occurrence, so the more accurate knock index, KI 20, was applied to the experimental data.

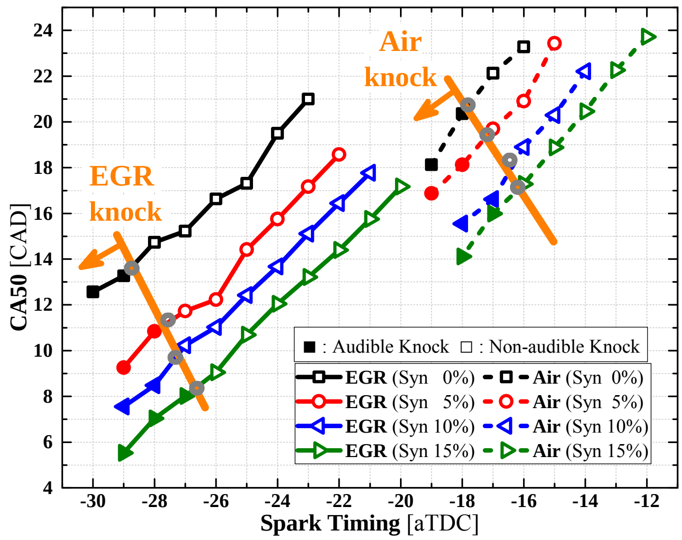


Figure 7. Results for spark timing and average CA50 for air and EGR dilution with and without syngas addition from the Hydra engine studies.

Figure 8 shows the knock intensity (natural log of KI 20 value) versus CA50 along with regression lines. The top and middle graphs show scatter plots of all knocking cycles under air dilution and EGR dilution, respectively. The knocking guideline is set to -5.298 (= ln (0.005)) based on the guideline of KI 20 (0.005 bar^2), and linear regression lines are extracted from the scatter points for each syngas amount. The bottom graph indicates the combined regression lines of both diluting conditions with error bars indicating the standard deviation. For advancing CA50, knock intensity linearly increased and the slope was similar for all cases.

Using the intersection of the regression lines and KI 20 knock guideline, the CA50 values at knock onset can be extracted (denoted by the grey circles in **Figures 7, 8,** and **9**). The CA50 values of knock onset were 13.4, 11.4, 9.6, and 8.4 at 0%, 5%, 10%, and 15% of syngas addition, respectively using EGR, and 20.7, 19.5, 18.3, and 17.2 at 0%, 5%, 10%, and 15% of syngas addition, respectively, using air dilution. From the results for CA50, it is clear that syngas addition was beneficial to knock mitigation based on combustion phasing.

In case of knock occurrence, for the comparison between EGR dilution and air dilution, the effect of syngas addition is represented by the CA50 of knock onset. For EGR dilution, the difference between syngas addition levels of 0% and 15% was 5.0 crank angle degrees, and for air dilution the difference was 3.5 crank angle degrees. Therefore, EGR dilution was almost 1.5 times more effective than air dilution for knock mitigation with syngas based on CA50 at boosted intake air conditions.

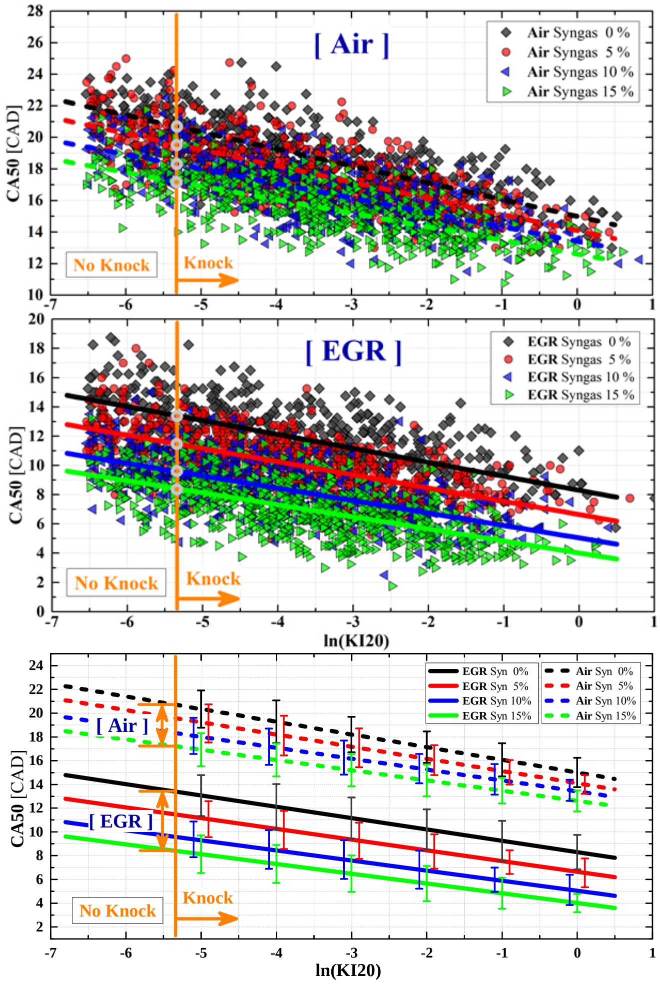


Figure 8. Results for knock intensity (natural log of KI 20) and CA50 from the Hydra engine studies for air and EGR dilution with varying levels of syngas addition. The lines are regressions to the different data sets.

Figure 9 indicates another criterion of knock, which is knock cycle percentage. This criterion was obtained by counting the number of knocking cycles over 200 cycles at the same test condition, where the knock guideline was also set to 0.005 bar^2 of KI 20. The knock cycle percentage proportionally increased with overall knock intensity. Based on the knock onset conditions identified from **Figure 7**, the percentage of knock-limited cycles was greater than nearly 65% and which is consistent with other engine studies.

The results of this project have established extensive understanding and data on the knocking characteristics for the Hydra engine facility. Knock extension studies are continuing using the Hydra engine facility leveraging this work and include combining multi-injection direct injection with PFI fueling.

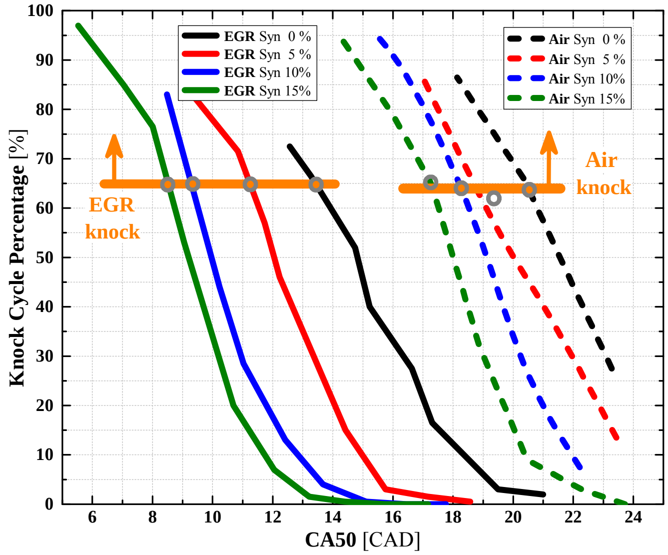


Figure 9. Results for average CA50 and knocking cycle percentage from the Hydra engine studies for air and EGR dilution with varying levels of syngas addition.

Task 1.3.2 Outcomes from the Single-Cylinder Ford Eco-Boost 0.33L Engine Facility

Using the single-cylinder Ford Eco-Boost engine facility, the effects of different fuel injection timing were studied as a function of ethanol and gasoline blend compositions, including the use of a one versus two fuel injection events for the different fuels. All fuel blends showed sensitivity to start of injection (SOI) timing, with efficiency decreasing with later injection timings. The results for gross indicated thermal efficiency (GITE) at maximum brake torque (MBT) spark timing for the different fuels and fuel injection timings are presented in **Figure 10**, for manifold absolute pressure (MAP) = 1 bar. The error bars in all figures are the standard deviations of the recorded combustion cycles, unless stated otherwise. In **Figure 10** the timing of the intake valve opening profile (IVOP) is provided for reference.

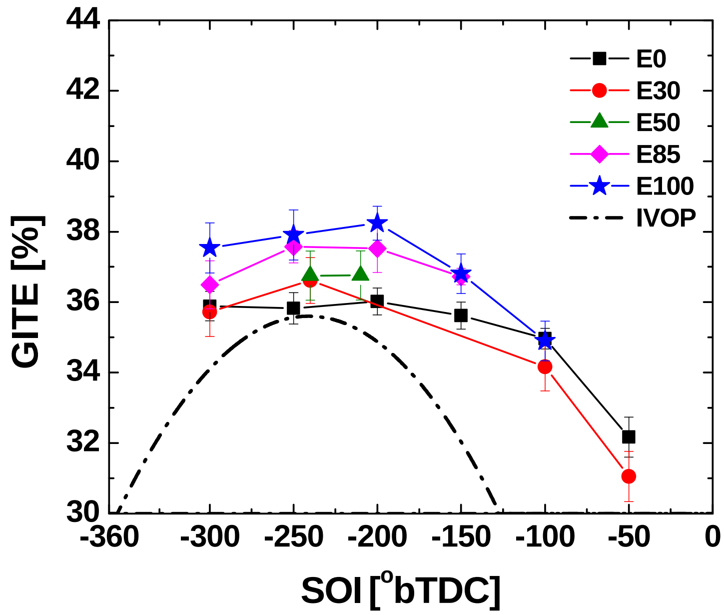


Figure 10. Results from the Ford Eco-Boost engine facility for GITE for single fuel injection events at MAP = 1 bar for different fuel blends. E0 = 100% reference grade gasoline fuel, E100 = 100% anhydrous ethanol fuel, E30 = 30% by volume ethanol, 70% gasoline, etc. IVOP = intake valve opening profile.

The ethanol fuel blends all yielded higher GITE compared with gasoline and no ethanol blend was limited by knock. The maximum GITE for all conditions was 38%. **Figure 11** compares the GITE for the fuels as a function of MAP. Since operation with E0 was limited by knock at the boosted intake air pressure conditions, the GITE was systematically lower for E0 compared with the ethanol blends. The efficiency for E0 also decreased as MAP increased as the spark timing was retarded further from MBT. **Figure 12** shows the CA50 (crank angle position where 50% of the total heat is released) for all the ethanol blends is around the MBT timing of 10° aTDC, whereas for E0 the CA50 was retarded by ~10° for the highest MAP conditions. The CA50 for E0 was more retarded with increasing MAP, which explains the trend of increasing offset of GITE between E0 and the ethanol blends observed in **Figure 11**.

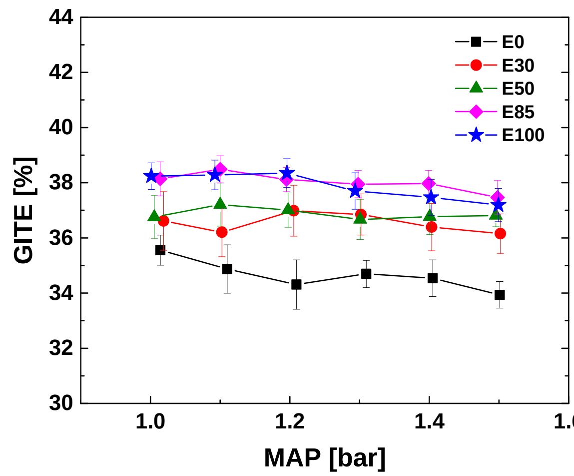


Figure 11. GITE results corresponding to the data presented in **Figure 10.**

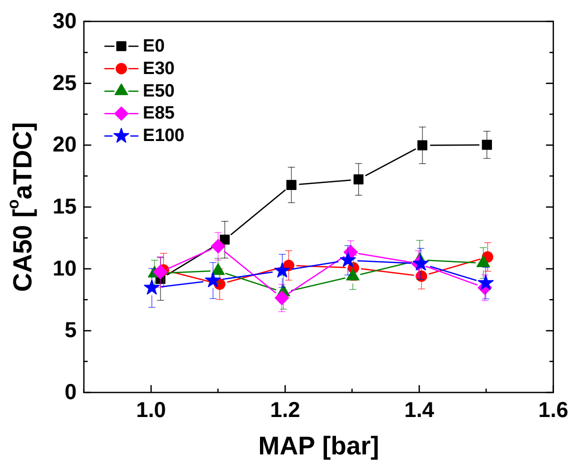


Figure 12. CA50 phasing corresponding to the data presented in **Figure 10.**

The effects of a binary fuel injection strategy, with equal fuel mass injected in each of the two injection events (SOI1 and SOI2) in each engine cycle, were studied for the fuel blends using the Ford Eco-boost Engine Facility. A split injection strategy with both injection events occurring during IVO was used in the study. The timing of the second injection event, SOI2, was kept in the range that led to maximum gross indicated mean effective pressure (GIMEP). Spark timing was kept the same for each fuel as identified in the single injection event study. **Figure 13** compares the results for GIMEP, GITE and Coefficient of Variance (CoV) of GIMEP for the single and split fuel injection operating conditions. The data show the split injection strategy resulted in comparable GIMEP, CoV, and GITE for all blends and MAPs. No significant benefit was observed to the binary fueling strategy in comparison with the single injection strategy based on these metrics.

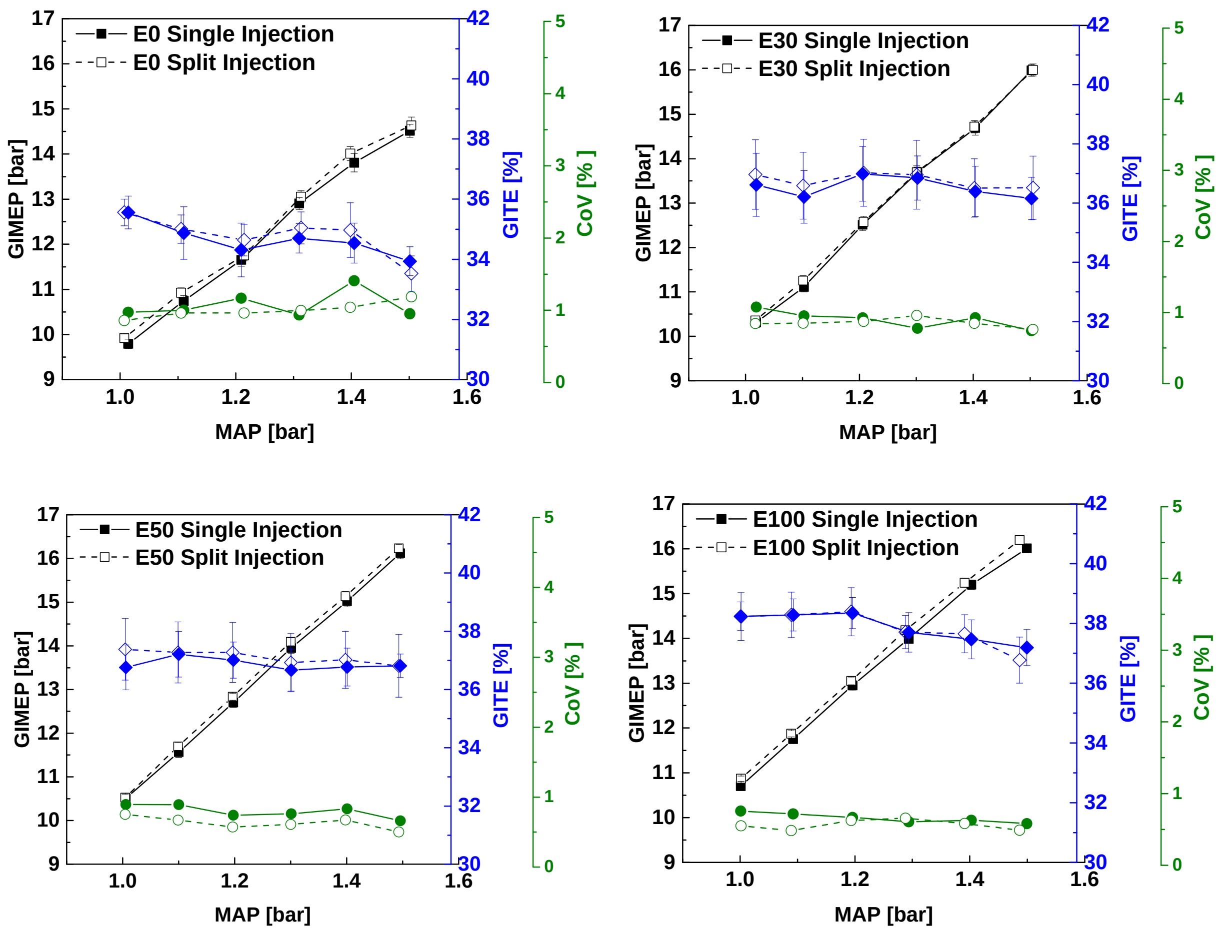


Figure 13. Comparison of GIMEP, CoV of GIMEP and GITE for single and binary fuel injection strategies using different ethanol and gasoline fuel blends.

A linear dependence on relative gain in GITE was observed as a function of mass fraction of the ethanol content in the fuel blend. This scaling supports the conclusion that effects of HoV were a significant factor controlling the thermal efficiency gains. This was confirmed by the GT power model simulation results presented above which showed that the efficiency gains with ethanol are partly due to HoV accounting, and partly due to beneficial effects of charge cooling. Another key conclusion of the study was the GIMEP and GITE of the different fuel blends showed little sensitivity to the split injection strategy relative to using a single fuel injection event. The lack of sensitivity was attributed to the limited range of SOI where the HoV of ethanol could positively impact the fuel air charge, i.e. during intake valve opening.

Task 1.4. Lean Spray Guided Multi-Cylinder Engine Studies to Extend Knock Limits and Mitigate PM/PN

The engine for the multi-cylinder work was a Daimler M274 2.0 L, 155 kW output engine with a piezo-crystal fuel injection system which was provided by Bosch, LLC as part of the cost-share commitment for the project. A large range of fuel injection strategies were explored as part of this work. A summary of the results of the study is currently in preparation for submission (Singh et al. 2017b).

The design of experiments for the multi-cylinder engine study was based on the learning outcomes of the single-cylinder Ford Eco-Boost engine study. Three fuel blends, up to four fuel injections per cycle (each with equal mass), four manifold absolute pressures and different SOI and pause/dwell times were studied. The range of conditions are listed in Table 4.

Table 4. Experimental Matrix for Daimler M-274 engine (Equal Fuel Mass split)

Fuel Blend Tested [Ethanol %]	E0	E30	E85				
Intake Pressure [mbar]	800	900	1000	1200			
Number of Injections	1	2	3	4			
Corresponding Fuel Split*	NA	1:1	1:1:1	1:1:1:1			
Start of Injection (SOI1) [dbTDC]	300	280	260	240	220	200	180
Pause/Dwell time for each SOI1 [CAD]	21	31.5	42	52.5	63		

The results for brake thermal efficiency (BTE) and coefficient of variance (CoV) of IMEP for different fuels and fuel injection timings, corresponding to MBT conditions at 800 mbar MAP, are presented in **Figure 14**. The error bars in all figures are the standard deviations of the recorded combustion cycles, unless stated otherwise. For MAP > 800mbar E0 fuel was limited by knock. It is observed that all three fuels behave similarly in terms of sensitivity to SOI timing. As we move towards later injection timing the BTE decreases and CoV increases; the performance with E85 fuel is the most adversely affected for later injection timing.

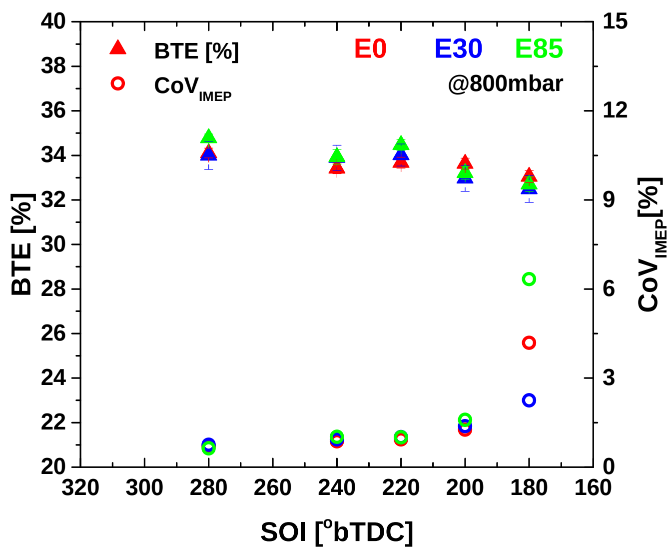


Figure 14. Comparison of BTE and CoV for different fuel blends as a function of SOI for single fuel injection events using the Daimler multi-cylinder engine facility for MAP = 0.8 bar.

Figure 15 presents the results for the BTE and CA50 for fuel blends at different intake pressures tested. BTE improves for E30 and E85 with increasing intake pressure whereas it falls for E0 fuel, similar to observations with single-engine cylinder studies. This observation is due to the limit posed by knock because of which E0 cannot be run at MBT timing above 800 mbar MAP. An absolute BTE improvement of 3% observed for E85 compared with gasoline within the range of MAP tested. It is also noted that the operation of engine above 1200mbar MAP is limited by pre-turbo exhaust temperatures with E0 fuel for stoichiometric operation, for E30 and E85 fuel blends though no knock or high exhaust temps are observed the operation above 1200 mbar is limited by peak-in cylinder pressures reached.

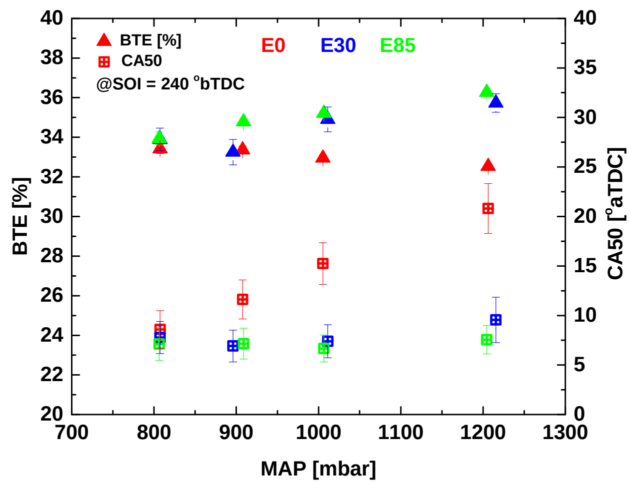


Figure 15: Comparison of BTE and CA50 for different fuel blends as a function of MAP for single fuel injection events using the Daimler multi-cylinder engine facility.

Figure 16 presents the results for the brake specific fuel consumption (BSFC) for the fuel blends at different intake pressures corresponding to the data presented in **Figure 15**. The results for BSFC were very sensitive to the ethanol content in the fuel. BSFC increased with increased ethanol content, due to the lower heating value of ethanol compared with gasoline. **Figure 16** captures how the lower levels of ethanol blends like E30 can become more attractive from a fuel economy aspect as the BSFC values for E30 approach those for E0 as at higher levels of MAP.

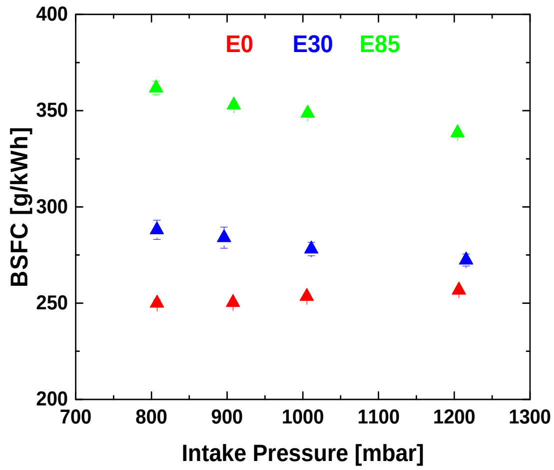
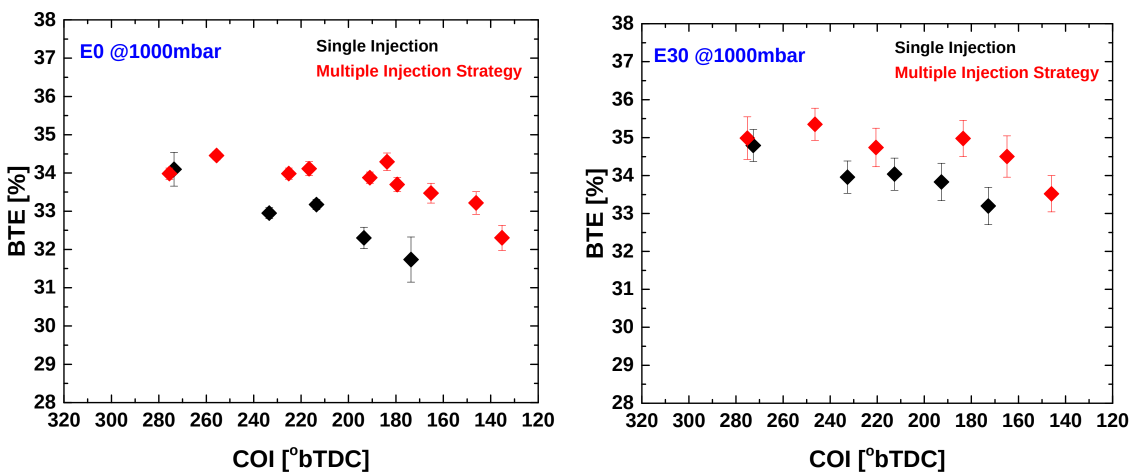


Figure 16. Comparison of BSFC for different fuel blends tested with single fuel injection events

The comparison between the baseline single and multiple injection event was facilitated by defining the center of injection (COI) timing, where COI is the center of the start of the first injection event and the end of the last injection event on a crank angle degree basis. **Figure 17** compares the BTE observed for single and multiple injection for MAP = 1 bar.



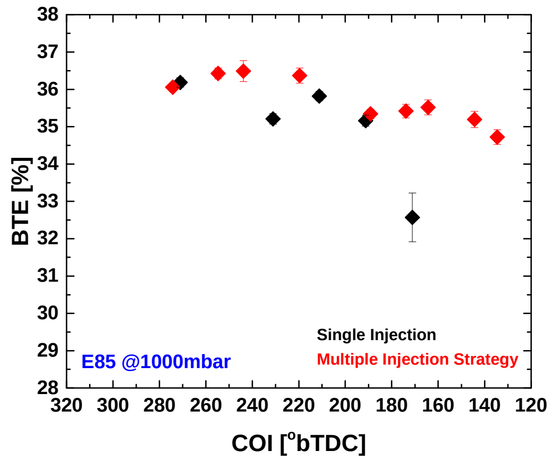


Figure 17. Comparison of BTE for single and multiple fuel injection event strategies for E0, E30 and E85 and at MAP = 1 bar using the Daimler multi-cylinder engine facility. Results for 2, 3 and 4 injection events are plotted together as "multiple injection strategy" strategy.

For earlier COI timing, the BTE was similar for the single and multiple injection event strategies. But as the COI was retarded and moved closer to TDC (and firing), the multiple injection strategy improved the BTEs for these stratified charge conditions. **Figure 18** shows a comparison of the results for the corresponding gaseous emissions (CO, THC and NO_x) for the E0 fuel conditions. Compared with the baseline single injection strategy, the multiple injection strategy lowered CO (15-25% reduction) and THC emissions and slightly increased NOx emissions. The improvement in BTE and lower CO as well as THC emissions with the multiple injections at later COI is attributed to improve homogeneity achieved with the use of multiple injections.

Several permutations of the fuel injection strategies were also studied, including varying the fuel mass in the different injection events. The impact on the engine performance including emissions are presented in **Figure 19**. The results show the ethanol blends systematically outperform E0 and multiple injection events can dramatically improve particulate, CO and THC emissions.

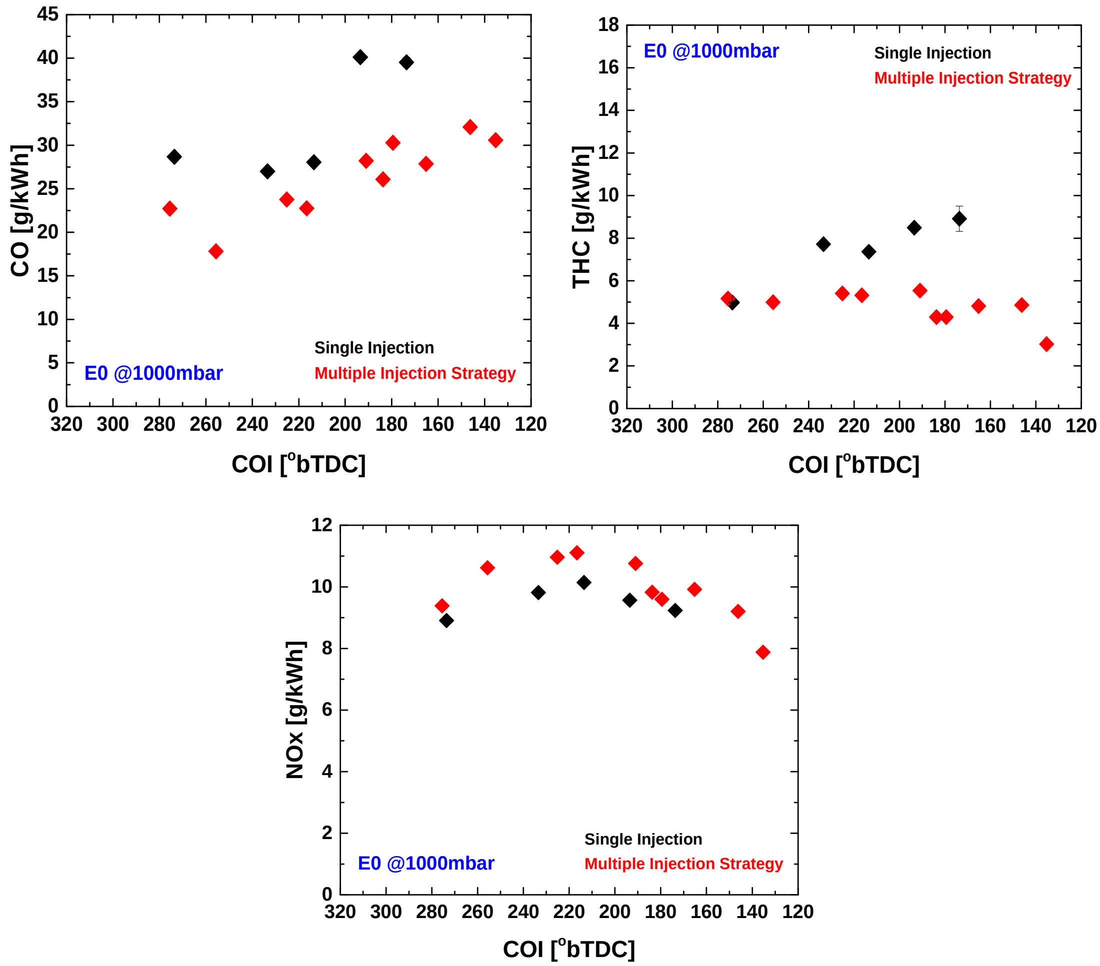


Figure 18. Comparison of CO, THC and NOx emissions for single and multiple fuel injection strategies for E0 fuel and MAP = 1 bar from the Daimler multi-cylinder engine facility study.

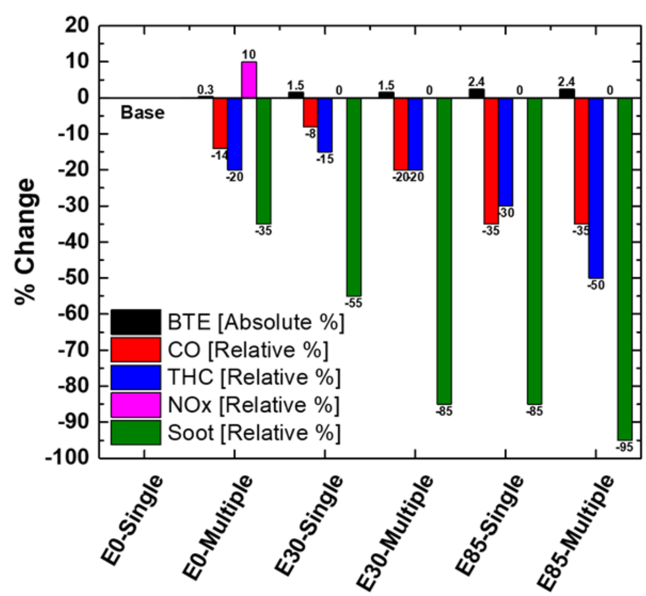


Figure 19. Comparison of the effects of the different fuels and injection strategies on engine performance for MAP = 1 bar.

Task 1.5 Dual Fuel Combustion for High CI Engine Efficiency

This task was meant to demonstrate 50% peak thermal efficiency at one speed and load condition in a new 1.9L turbodiesel test engine and pursue extension of the operating range and optimization of the combustion strategy. Much of the first year of the project was devoted to configuration of the dual fuel delivery system, using an intake fumigator developed for prior DOE-sponsored work and a DME and propane delivery system to provide high accuracy control and delivery of the liquefied gaseous fuels. The last quarter of Year 1 was devoted to the dual fuel combustion research activity. **Figure 20** presents a sample of the matrix of test results. Unfortunately, the results from the completed test facility demonstrated little to no improvement in thermal efficiency over the baseline of conventional diesel combustion. As we could not meet the Go/No Go decision point, this task was discontinued.

During the course of experiments, we explored the dual fueling strategy using liquefied gas mixtures of DME and propane over a broad range of compositions and engine operating conditions. We extended previous test conditions to high speed and load and evaluated substitution of diesel by the fumigated gas mixtures up to 70% on an energy basis. We evaluated the resulting engine behavior through heat release analysis, BSFC and emissions measurements and performed a statistically based optimization of the fueling strategy over the range of engine conditions tested, working with two Automotive Engineering MS students for their Auto 503 capstone design project. The work led to follow-on support from an industrial sponsor, as an outcome from this DOE project.

As part of the work we conducted testing to identify an optimal level of diesel substitution (including variation of the injection strategy for the diesel fuel itself, using lessons learned in the studies of reactivity controlled compression ignition, reactivity controlled compression ignition (RCCI) combustion, and DME/propane ratios to attempt to optimize the dual fuel combustion. Overall, we were not able to reproduce the extent of thermal efficiency improvement that we observed previously, and never got close to 50% BTE.

The work performed under this task, while unsuccessful in meeting the objectives of the present DOE funded program, has served to support other DOE sponsored activities. Test engine mapping was performed and experiments were completed for DOE-Volvo ***Supertruck 1***, for which UM was a subcontractor to explore the potential of post injection strategies to mitigate particulate emissions via control over in-cylinder soot formation and oxidation (Martin et al., 2016). Testing of the optimal level of diesel substitution and DME/propane ratio was conducted. Building on the outcomes, a novel scheme was devised for bridging between pure RCCI combustion modes and conventional diesel combustion (CDC) modes (Martin et al., 2017). This involves using combinations of diesel injection strategy and DME+propane blending levels to achieve optimized combustion and emissions during the traverse from RCCI to CDC and back. Hino Motors is now supporting continuing work on this subject. In addition, a doctoral student used the test engine for studies of the impact of PCCI combustion, PCCI fuel formulation and post injection strategies on soot nanostructure and reactivity for her doctoral thesis which was defended in summer 2017. That former student now works for Volvo Technology of America in Hagerstown, MD.

	Conv.	20% Premixed 0%	20% Premixed 10%	20% Premixed 20%	40% Premixed 0%	40% Premixed 10%	40% Premixed 20%	60% Premixed 0%	60% Premixed 10%	60% Premixed 20%	
BTE	37.3%	36.2%	36.6%	36.7%	35.7%	36.2%	36.1%	36.5%	36.4%	36.9%	50% DME
		36.3%	36.3%	36.5%	34.9%	35.5%	35.7%	33.2%	34.9%	35.5%	33% DME
		35.9%	36.2%	36.5%	34.5%	35.5%	35.5%	29.9%	33.4%	34.8%	17% DME
CO, ppm	285	1605	1444	1290	3344	2775	2390	3040	3085	2779	50% DME
		1416	1293	1184	2719	2407	2078	4593	3414	2782	33% DME
		1295	1223	1113	2387	2121	1895	3732	3123	2581	17% DME
THC, ppm	216	856	804	717	1220	1146	1063	1329	1187	1116	50% DME
		1154	980	912	2008	1793	1567	3056	2356	1939	33% DME
		1389	1233	1065	2659	2272	1911	5264	3548	2704	17% DME
Comb. Eff.	99.1%	95.7%	96.1%	96.5%	91.8%	93.0%	93.8%	92.0%	92.4%	93.1%	50% DME
		95.5%	96.0%	96.3%	91.5%	92.5%	93.5%	85.7%	89.5%	91.5%	33% DME
		95.3%	95.7%	96.2%	90.9%	92.2%	93.2%	83.1%	87.8%	90.4%	17% DME
FSN	0.487	0.413	0.503	0.502	0.401	0.532	0.559	0.377	0.497	0.593	50% DME
		0.290	0.367	0.389	0.120	0.274	0.371	0.048	0.225	0.419	33% DME
		0.203	0.280	0.325	0.071	0.144	0.218	0.018	0.056	0.174	17% DME
NOx, ppm	612	510	527	525	387	409	407	317	356	366	50% DME
		528	556	534	458	439	426	335	352	341	33% DME
		543	560	554	450	479	465	259	370	376	17% DME
	6949	6984	7092	7070	7010	7074	6998	7530	7587	7495	50% DME
		6921	7101	7065	6590	6921	6909	6041	6880	7050	33% DME
		6912	7101	7067	6415	6734	6841	5462	6032	6612	17% DME
SD Peak Pres., kPa	54	42	43	44	43	38	39	164	83	55	50% DME
		43	51	48	50	56	52	98	67	55	33% DME
		44	51	53	44	63	64	55	68	84	17% DME
Max. PRR, kPa/CAD	835	819	717	696	722	440	412	509	432	369	50% DME
		940	836	803	867	759	650	623	583	437	33% DME
		1023	930	865	881	855	805	492	592	605	17% DME

% of premixed fuel energy from DI diesel squish conditioning pulse

Figure 20. Table of combustion and emissions results from the dual fuel combustion process. Variation in pilot and main diesel fuel injection, over range of pilot injection from 0 – 60% of diesel fuel injection on an energy basis, with variation in the DME content (up to 50% on energy basis) and propane content (up to 20% on energy basis). Compared to the conventional combustion condition, coloring in the table indicates whether the measured variable was better (green), similar (yellow) or worse (orange to red).

Products developed

1. Taehoon Han, George Lavoie, Margaret Wooldridge, André Boehman, (2017) "Effect of Syngas (H_2/CO) on SI Engine Knock under Boosted EGR and Lean Conditions," presented at the 2017 SAE World Congress, Detroit, Michigan, SAE Technical Paper No. 2017-01-0670 (2017).
2. Singh, R., Fatouraie, M., Burch, T., Lavoie, G., A., Wooldridge, M. S., (2017a) "Effects of Fuel Injection Events of Ethanol and Gasoline Blends on Boosted Direct-Injection Engine Performance," presented at the SAE 2017 Fuels and Lubricants Meeting, Beijing, China, SAE Technical Paper 2017-01-2238..
3. Singh, R., Han, T., Fatouraie, M., Wooldridge, M. S., Boehman, A., (2017b) "Effects of Fuel Injection Events of Ethanol and Gasoline Blends on Boosted Multi-Cylinder Direct-Injection Engine Performance," in preparation.
4. Middleton, R (2018) "Voronoi Partitions for Assessing Fuel Consumption of Advanced Technology Engines: An Approximation of Full Vehicle Simulation on a Drive Cycle", Submitted for the 2018 SAE World Congress, Detroit Michigan.

Modeling Information

a. Model description, key assumptions, version, source and intended use;

Commercially available software was used in the project as follows:

- CHEMKIN software [1] was used to compute the occurrence of knock in the end-gas under prescribed pressure-time histories for various fuel blends. The kinetic mechanism employed was the 312 species gasoline surrogate mechanism of Mehl et al. [2-3], which includes an ethanol sub-mechanism.
- GT-Power [4] was used to investigate the effect of fuel evaporation during intake and high heat from ethanol blends on fuel economy and heat loss.

b. Performance criteria for the model related to the intended use;

CHEMKIN was used to investigate relative behavior; no special calibration beyond normal engine thermodynamics was employed. The kinetics mechanism was unmodified from the version described by the originators. The GT-Power model was calibrated in a normal manner to match engine efficiency at a base point, after which only relative effects were studied.

c. Test results to demonstrate the model performance criteria were met (e.g., code verification/validation, sensitivity analyses, history matching with lab or field data, as appropriate);

See item b, above.

d. Theory behind the model, expressed in non-mathematical terms;

The CHEMKIN kinetics calculation is intended to represent the chemical history of a representative packet of end-gas which follows the prescribed pressure-time behavior observed experimentally or calculated using a suitable engine thermodynamic model such as GT-Power. The latter model is based on a two zone dynamic thermodynamic calculation representing burned and unburned gas history separated by the evolving flame front. It also has provision for modeling the evaporation process during injection of the fuel during the intake process.

e. Mathematics to be used, including formulas and calculation methods;

See references [1, 4]

f. Whether or not the theory and mathematical algorithms were peer reviewed, and, if so, include a summary of theoretical strengths and weaknesses;

These models have been peer reviewed numerous times and are the foremost recognized tools used by those skilled in the art of engine and kinetics modeling.

g. Hardware requirements;

Typical professional level personal computers are sufficient.

h. Documentation (e.g., users guide, model code).

See refs [1, 4]

Modeling Information References

1. CHEMKIN Chemical Reaction Software, Reaction Design, Inc., San Diego, CA.

2. Mehl, M., Chen, J. Y., Pitz, W. J., Sarathy, S. M., and Westbrook, C. K. (2011) An Approach for Formulating Surrogates for Gasoline with Application toward a Reduced Surrogate Mechanism for CFD Engine Modeling. Energy Fuels, Vol. 25, No., 5215–5223,

3. Mehl, M., Pitz, W. J., Westbrook, C. K., and Curran, H. J. (2011) Kinetic modeling of gasoline surrogate components and mixtures under engine conditions. Proceedings of the Combustion Institute, Vol. 33, No. 1, 193-200, doi:http://dx.doi.org/10.1016/j.proci.2010.05.027.

4. GT-Power Engine Simulation Tool, Gamma Technologies Inc.

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