Report 15: Cost-Effective Reciprocating Engine Emissions Control and Monitoring for E&P Field and Gathering Engines

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Author
Kirby S. Chapman, Ph.D., Kansas State University
Sarah R. Nuss-Warren, Research Associate, Kansas State University

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Kansas State University
National Gas Machinery Laboratory
245 Levee Drive
Manhattan, KS 66502

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Abstract
Continuing work in controlled testing uses a one cylinder Ajax DP-115 (a 13.25 in bore × 16 in stroke, 360 rpm engine) to assess a sequential analysis and evaluation of a series of engine upgrades. As with most of the engines used in the natural gas industry, the Ajax engine is a mature engine with widespread usage throughout the gas gathering industry. The end point is an assessment of these technologies that assigns a cost per unit reduction in NOX emissions.

Technologies including one pre-combustion chamber, in-cylinder sensors, the means to adjust the air-to-fuel ratio, and modification of the air filter housing have been evaluated in previous reports. Current work tests non-production, prototype, mid-pressure fuel valves and begins analysis of these tests. This analysis reveals questions which must be answered before coming to any firm conclusions about the use of the 180 psig fuel valve. The research team plans to continue with the remaining pre-combustion chamber tests in the coming quarter. By using the Ajax DP-115 these tests are completed in a low-cost and efficient manner. The various technologies can be quickly exchanged with different hardware, and it is inexpensive to run the engine.

Progress in moving toward field testing is discussed, and a change in strategy is suggested. Although field engines are available to test, it is suggested that the final field testing be put on hold due to information from outside publications during this last quarter. Instead, KSU would focus on related field-testing and characterization in an outside project that will close an apparent technology gap. The results of this characterization will give a more solid footing to the field testing that will complete this project.
Table of Contents

Disclaimer..................................................................................................................... i

Abstract .......................................................................................................................... ii

Table of Contents............................................................................................................ iii

Introduction ...................................................................................................................... 1

Basis of the Project .......................................................................................................... 3

Controlled Tests ............................................................................................................ 4

Data Acquisition Improvement .................................................................................... 5

Mid-pressure Valve Tests.............................................................................................. 5

Field Testing .................................................................................................................... 8

Conclusions and Future Work ....................................................................................... 11

Acknowledgements ........................................................................................................ 11

References ...................................................................................................................... 12

Appendix A: Data Analysis............................................................................................. 13
  (a) Average Cylinder Peak Pressure ............................................................................... 13
  (b) Average Standard Deviation of Cylinder Peak Pressure .............................................. 13
  (c) Brake Specific Fuel Consumption ............................................................................. 14
  (d) Trapped Equivalence Ratio ....................................................................................... 15
  (e) Emissions.................................................................................................................. 16

Appendix B: Additional Data ........................................................................................ 19
Introduction

The objective of this project is to identify, develop, test, and commercialize emissions control and monitoring technologies that can be implemented by exploration and production (E&P) operators to significantly lower the cost of environmental compliance and expedite project permitting. The project team will take considerable advantage of the emissions control research and development efforts and practices that have been underway in the gas pipeline industry for the last 12 years. These efforts and practices are expected to closely interface with the E&P industry to develop cost-effective options that apply to widely-used field and gathering engines, and which can be readily commercialized.

The project is separated into two phases. Phase 1 work establishes an E&P industry liaison group, develops a frequency distribution of installed E&P field engines, and identifies and assesses commercially available and emerging engine emissions control and monitoring technologies. Current and expected E&P engine emissions and monitoring requirements will be reviewed, and priority technologies will be identified for further development. The identified promising technologies will be tested on a laboratory engine to confirm their generic viability. In addition, a full-scale field test of prototype emissions controls will be conducted on at least ten representative field engine models with challenging emissions profiles. Emissions monitoring systems that are integrated with existing controls packages will be developed. Technology transfer/commercialization is expected to be implemented through compressor fleet leasing operators, engine component suppliers, the industry liaison group, and the Petroleum Technology Transfer Council.

Forecasts of future U.S. natural gas demand of 30 trillion cubic feet (Tcf) /yr by 2015 require 36% production growth from 2001 levels. Demand growth will be addressed by both conventional gas and coal-bed methane. The majority of the increase in conventional gas production is expected from three primary areas: Offshore Gulf of Mexico, Rocky Mountains, and Canadian imports. Mature basins in the Southwest and Mid-Continent areas will also contribute to the total domestic supply, and maximizing their output will be necessary to meet the aggressive 30 Tcf gas demand target.

Oil and gas production operations in the United States face a wide variety of environmental regulations that are imposed by multiple, sometimes overlapping, jurisdictions. In particular, onshore production must grapple with existing and emerging regulations that address National Ambient Air Quality Standards for ozone, fine particulates, and NO₂, regulations regarding acid deposition and regional haze, and pending air toxics regulations, all of which will limit emissions from compressor engines. NOₓ and formaldehyde will be the likely focus. The scope of these regulations will include the assessment of the need for emissions controls on the wellhead and field gathering reciprocating engine-driven compressor and pumping equipment that is ubiquitous in E&P operations. Current estimates are that approximately 15 million horsepower are presently operating in upstream production applications (Hanover Compressor Company 2001 10-K Annual Report filing). At an average size of 250 HP, this implies a total E&P fleet of 60,000 engines.

Though in many oil and gas production areas the air shed emissions inventory is dominated by coal power plants, regulatory agencies continue to pursue incremental reductions in total
pollutant loading. Reciprocating engines have been identified as a meaningful source category. This is evident in Federal and State actions, as well as Environmental Impact Statements associated with new development. These engines are used to produce electricity for a leasehold, compress and re-inject natural gas for increased oil production, compress natural gas so that it can be delivered to local gathering systems that ultimately feed into gas transmission pipelines, and drive smaller-load equipment such as pump jacks.

At present, the region with the greatest confluence of emissions concerns for small IC engines is the Rocky Mountain and Intermountain West area. In these regions, significant concerns about regional haze control accelerated the implementation of NOₓ and fine particulate regulations that are only pending in many other producing areas. However, the incremental adoption of regulations state-by-state, as well as the proximity of many remote production areas in the Southwest to National Parks and Class I Wilderness Area (which are protected air-sheds) may likely stimulate aggressive compressor engine controls in that and other production regions, as well. Finally, the East Texas and Louisiana regions are subject to conventional ambient ozone concerns, and have promulgated strict NOₓ controls for reciprocating engines. In addition, EPA will propose regulations in 2006 for final adoption in 2007 that will address smaller IC engines in all applications throughout the U.S. These rules include a New Source Performance Standard for IC engine, as well as air toxics standards for: (1) area sources (i.e., engines at smaller facilities), and (2) 500 hp and smaller engines at major sources.

Oil and gas production from all states will be required for the U.S. to meet the expected 30 Tcf/year gas demand and to minimize the ongoing slide in domestic oil production, and impediments to production that are created by air quality permitting must be alleviated through focused R&D efforts.

Gas compressor operations are an essential element of oil and gas production. Increased emissions constraints on compressor operations affects oil and gas production in four distinct ways:

- The length of time to obtain an emissions permit is increased as multiple jurisdictions evaluate the effects of various pollutants and attempt to define a mutually acceptable permit level for a given engine. Furthermore, permitting may become impossible when performance targets for application of emission controls to small engines are inappropriately established at levels that are technically infeasible or only achievable based on expenditures well in excess of forecasts of the implementing agencies.

- The capital and operating costs of compressor engine operation are increased as this equipment is physically modified and/or operated differently to comply with the air permits.

- The capital and operating costs of compressor engine operation are increased when expensive and maintenance-intensive continuous emissions monitors are required, as is the case in parts of California. In many settings, the cost of this monitoring exceeds the cost of NOₓ control.

- Compressor operators may be forced to limit the annual hours of operation to avoid exceeding a fixed annual ceiling on allowed emissions.
Each of these situations impedes oil and gas production by:

- Deferring the start of wellhead production, thereby increasing the general business risk in current price-volatile markets and increasing the carrying costs of various lease and development fees;
- Directly increasing the cost of compression services used at the wellhead; and
- Artificially limiting the annual take from a well due to constrained operations.

The net effect is reduced oil and gas production for a given cost within a fixed time period. Multiplying this through thousands of production sites will most certainly have a significant negative impact on the ability of U.S. operators to meet domestic energy demands, and on the general productivity of the U.S. hydrocarbon resource base.

In addition, application of controls may result in emissions tradeoffs that can result in other deleterious environmental effects if not properly considered. These issues may be exacerbated by presumptions of technology performance that have not been proven for the engine sizes or operating applications present in oil and gas operations.

These economic and operating burdens to oil and gas operations can be reduced through a focused effort to develop cost-effective retrofit components, engine combustion controls, and engine performance monitoring options. The proposed project will significantly improve the cost-effectiveness of implementing NOX and formaldehyde controls and monitoring on compressor engines, while characterizing emissions tradeoffs – thus ensuring that compliance with air regulations does not prevent oil and gas operations from achieving their maximum productivity at competitive production costs.

**Basis of the Project**

This project draws heavily on the experience gained from the interstate gas pipeline industry’s experience with NOX emissions reductions, and their efforts to develop cost-effective options for extensive deployment throughout their systems. A number of gas pipelines faced EPA statutory deadlines in 1994/1995 to achieve and certify dramatic reductions in compressor engine NOX emissions across a very wide range of ageing and diverse, but critical, equipment. Even though typical pipeline reciprocating compressor engines range in size from 600 hp to 8,000 hp and are largely two- and four-stroke cycle integral compressors, there is some commonality in equipment types and operational concerns with the wellhead and gathering facilities under study in this project. Beginning in 1990, the pipeline industry embarked on a comprehensive R&D program that targeted significant (50%+) reductions in the cost of NOX controls without any significant engine performance compromises. All of the technologies developed had to be field-retrofitable and commercially-supported. That program was a significant success and created a number of technical options that allowed up to 80% NOX reductions in a cost-effective and operationally-acceptable manner. The individuals involved with this current project were key participants in that prior pipeline NOX and formaldehyde reduction program.

The gas pipeline emissions control technology development effort was instructive in that it employed the following six distinct phases of activity, each of which was necessary for success:

- Obtain an industry consensus for
• specific engine types and models on which to focus development efforts,
• installed cost targets,
• realistic emissions levels to be achieved under all operating conditions.

• Develop an inventory of installed horsepower to confirm initial industry guidance and to create a useful tool for impact analysis;

• Create a coordinated, core team of engine technologists, regulatory experts, and industry representatives to ensure that engine design issues, regulatory drivers, and practical operating considerations always were addressed simultaneously;

• Aggressively field test component and controls developments;

• Characterize the fundamental relationships between engine operating parameters and exhaust emissions so that accurate, non-instrumented emissions monitoring systems could be deployed; and

• Transfer technology results to organizations with an existing presence in the industry so that equipment could be provided on commercial terms, with emissions guarantees, and supported on an ongoing basis.

This project followed a similar broad outline with the expectation that the end product is a set of cost-effective emissions control and monitoring options that can be applied to a wide range of compressor engines in common use in oil and gas production. Operators will enjoy reduced costs of compliance, greater permitting certainty, reduced costs of emissions monitoring, and possible improved compressor performance due to improved combustion stability. All of this will sum to increased production as wells are brought online more rapidly, compression equipment is run harder and longer to facilitate increased production, and lifting cost savings are reallocated toward additional resource base development.

## Controlled Tests

Controlled tests are conducted on the Ajax DP-115 at Kansas State University to address a series of upgrades intended to improve emissions. The DP-115 is a mature two-stroke cycle lean burn (2SCLB) engine, typical of those found at gathering sites. While many technologies have already been tested, more remain. Progress in controlled testing during this quarter included significant improvement of the data acquisition system, testing on a mid-pressure fuel valve, and analysis of data from this testing.
Data Acquisition Improvement

This quarter, the data acquisition system for the Ajax was completely overhauled. The data acquisition hardware had previously been operating in an open rack. This left electronics open to dust and debris. Another concern was that electrical terminals were open to lab personnel, which could have been a safety hazard. The donation of a large, enclosed cabinet from Exline, Inc. enabled the data acquisition system to be enclosed (Figure 1). Additionally, permanent cables replaced temporary cables that had previously been disconnected after every run. This change has improved data and instrument reliability. For instance, the dyno controller has been holding its calibration more reliably since the change. Finally, a control algorithm was programmed into the data acquisition system to check for conditions that could damage equipment or, even worse, harm lab personnel. This was especially important considering the addition of high pressure natural gas on-site. The control algorithm was designed to check for over-temperature, over-pressure, over-load or over-speed conditions as well as coolant flow on the engine and dyno. If a limit is exceeded, the control algorithm automatically shuts off the equipment.

Mid-pressure Valve Tests

Tests were conducted using a 180-psig, electrically controlled, pneumatically actuated, non-production, prototype fuel valve. Emissions data was collected from 75% of full load (1200 ft-lbs) to 99% of full load (1600 ft-lbs) for each of three speeds (300, 330, and 360 rpm) over the operating range at three settings of ignition timing (8°, 11°, and 14° BTDC). The engine was allowed to stabilize for 20 minutes after any change to speed or load before a data point was collected. Timing was changed at the beginning of the day, as the engine must be off to change the timing. A total of 38 data points were collected. Each point consisted of emissions measurements in ppm of CO, NO, NO₂, and O₂. At each point, engine parameters including speed, applied load, fuel flow, temperatures and pressures for fuel, intake and exhaust, and
ambient conditions were recorded each second for five minutes. Additionally, high speed data was taken every 0.1° for in-cylinder pressure, ion current, and intake and exhaust pressure for five minutes.

The parameters that give insight into the effectiveness of any emissions control strategy must clarify how well the engine runs as well as showing emissions produced per unit work done by the engine. Average peak pressure, the standard deviation of cycle-to-cycle peak pressure, and brake-specific fuel consumption characterize engine performance using this mid-pressure prototype valve. The equivalence ratio, which is changed by adjusting the load and speed (Figure 2), has a direct impact on the amount of NOX that will be produced in each cycle. Each of these parameters is calculated from the data collected during the tests, with calculations shown in Appendix A.

As the in-cylinder trapped air-to-fuel ratio becomes leaner, the misfire frequency tends to increase. Thus, there should be a decrease in standard deviation of peak pressure, which indicates an increase in combustion stability, as the trapped equivalence ratio increases toward one. This is true for each speed line in the 8° before top dead center (BTDC), 11° BTDC, and 14° BTDC data (Figure 3). However the 11° BTDC data has more scatter than the 8° and 14° data for standard deviation of peak pressure.

Production of NOX depends on the rate of the chemical reaction that takes atmospheric nitrogen and unused oxygen to NO and takes NO and additional unused oxygen to NO2. This rate depends on the trapped equivalence ratio, time allowed for the reaction to occur, and temperature [1]. As equivalence ratio for a lean burn engine increases toward unity, which gives a stoichiometric air-to-fuel ratio, temperatures tend to increase as well. The time in which the reaction can happen is determined by the engine speed. In this case, the trapped equivalence ratio does not depend on speed due to the particular aspiration mechanism in an Ajax engine. For a single equivalence

![Trapped Equivalence Ratio at 14° BTDC](image)

**Figure 1.** Typical data from the mid-pressure valve test.
ratio, as speed increases, NOX decreases (Figure 4). Similarly, it is expected that as equivalence ratio increases, the NOX produced should also increase. However, since the equivalence ratio is increased by adding load, the specific emissions are actually lower for high-power runs (Figure 4), even though the equivalence ratios may be higher in some cases. Specific CO production is lower for higher equivalence ratios (Figure 5).

Figure 2. Engine stability based on peak pressure.

Figure 3. At 8° BTDC, specific NOx as a function of engine speed and trapped equivalence ratio.
Both NOX and CO were calculated using the exhaust flow and exhaust molecular mass determined through a carbon balance beginning with the basic chemical reaction for combustion (Appendix A). This is slightly different from the EPA’s Method 19. Because most of the NOx produced in these runs is NO, Method 19 would overestimate the total mass flow rate of NOx by almost 50%. This is because Method 19 uses a single density [2, 3], that of NO2, for both NO and NO2 in the calculation of mass flow rate. The mass of NO2 is 16 atomic mass units greater than that of NO, which is about half the mass of NO and one-third the mass of NO2. Currently, no corrections have been applied for ambient conditions.

One concern about this data is the failure of some of the collected data to segregate into speed lines (Figure 6). As discussed above, NOx formation should depend on engine speed, and so data is expected to follow segregate into speed lines as in Figure 4. This issue requires additional analysis and investigation before any conclusions can be drawn. After additional analysis, a cause may be determined for this anomaly which confirms the remaining data, or it may be decided that more data needs to be collected in order to come to a firm conclusion regarding the effectiveness of the 180-psig valve for emissions control. Additional graphs showing this behavior, as well as other additional graphs, are located in Appendix B.

### Field Testing

The goal of the field testing phase is to provide a robust data set from engines operating over a wide range of conditions to confirm that the laboratory tested technologies are effective in the field. The research team hopes to gain consistent field data. Good field data will not only demonstrate the success of the selected control technologies, but allow the research team to characterize the fundamental relationships between the engine operating parameters and the exhaust emissions. This characterization would prove highly useful to the industry, as it would allow non-instrumented or less heavily-instrumented emissions monitoring, which would meet the goal of a low cost solution.

**Figure 5.** At 8° BTDC, specific CO as a function of engine speed and trapped equivalence ratio.
In order for the data set to be truly robust, sufficient in-house testing must be finished. For the two-stroke lean burn engine, in-house testing progresses as described above, but is not yet finished. For the four-stroke rich burn engines, it was widely accepted in the industry that the solution to solving emissions is to add a NSCR catalyst and air-to-fuel-ratio controller. The research team planned to use this technology for field tests on the four-stroke-cycle rich burn engines [4]. When the initial testing was completed by AETC for the rich burn engines, the conclusion was that catalysts at that time were not the ultimate solution to NOx control. Reasons for this conclusion include the need for a catalyst break-in period and the resulting need to make frequent air-to-fuel ratio set point adjustments, lag in catalyst response, and insufficient monitoring capabilities to determine if the catalyst is working [5]. However, due to wide industry acceptance of catalysts as the solution to control emissions on rich burn engines, the research team determined that a catalyst and full authority air-to-fuel-ratio controller would be the proper technology to demonstrate emissions control for four-stroke-cycle rich-burn engines [6].

Late this quarter, several events precipitated a change in the research team’s strategy regarding field testing for four-stroke rich-burn engines. One major concern is that limits are continually increasing their scope. In the Four Corners area and Wyoming, focus is shifting to ever-smaller engines. Engines under 150 hp are expected to face considerable regulations in this area over the course of the next year or so [7]. Small horse-power units form a particularly large portion of the gathering industry’s engines. The industry is looking for a solution that will apply well to these smaller engines. Additionally, a project involving monitoring systems fitted with catalysts was completed in the South Coast Air Basin of California [8, 9]. The results indicate that more four-stroke cycle research needs to be done before field testing will yield data that can be used as the KSU research team hopes.

The southern California researchers found emissions excursions for only about 5% of the periodic monitoring tests done over a 13-week period on well-maintained systems “as found.” In
this case, “as found” means that these systems had been operating using a given NSCR catalyst and air-to-fuel-ratio controller for the long term and had been well tuned and passed initial catalyst break-in before this test began. For four of the six units in this study, emissions limits were the higher Best Available Retrofit Control Technology (BARCT) rather than the super-low limits for Best Available Control Technology (BACT) of 0.15 g/bhp-hr NOx and 0.6 g/bhp-hr CO. Despite the relatively few excursions, the researchers found the alarms systems on the controllers were insufficient for predicting or detecting the excursions that did occur. Many excursions seem to have been caused by operational issues, such as the need for A/F set point adjustments, ineffective oxygen sensors, clogged catalyst, or fouled sensors. Reasons for excursions on the two BACT engines were generally unknown, though unusual ambient conditions contributed to one excursion [8].

The other part of the South Coast project, which provided continuous monitoring to systems using various controllers, demonstrated serious issues in catalyst control. One engine had been retrofitted for BARCT levels, but the researchers attempted to run it at BACT levels with the various air-to-fuel-ratio controllers. Although the unit achieved BACT levels at some times, it could not maintain BACT levels because the catalyst did not have sufficient oxygen storage to deal with changes in ambient conditions. In general, none of the tested engines, even the unit that was originally designed to meet BACT criteria, was able to stay in compliance during continuous testing. Changes in ambient condition, emissions spiking, and difficulty in effectively programming the air-to-fuel-ratio controller all contributed to difficulties in keeping the engines in compliance. Additionally, the alarms in the air-to-fuel-ratio controller were insufficient to recognize the excursions from the very low emissions limit [9].

The implications of the results of the California tests combined with emissions limits’ expansion to cover smaller engines are significant. Even small changes in ambient conditions are expected to cause major drifts in emissions. Standard operation reveals emissions spiking, catalyst lag, and lack of effective alarms. To get data that will allow enough modeling to create less-heavily-instrumented monitoring systems, the research team will need to test emissions systems that produce consistent results. Current controls systems do not meet this criterion [8, 9]. Therefore, more testing is needed before field testing for this project can commence.

Fortunately, industry intends to fund further research into NSCR catalyst operation. The KSU research team plans to work with a number of gathering companies, including BP, to collect data for various small horsepower four-stroke-cycle rich-burn engines in the Four Corners area over the next year to 14 months. Up to about 10 engines will be outfitted with NSCR catalysts and air-to-fuel-ratio controllers. Their running conditions and emissions will be monitored semi-continuously for an entire year. The data will be used to determine what the limits of effectiveness are on the catalysts. Likely, improved control algorithms and alarm conditions will be developed. After this data has been collected, the KSU research team will run several of the catalyst-fitted engines for an additional 10 months of mapping. At this time field testing of other engines will begin, as well. The mapping data will be used in this project and submitted to the Department of Energy and to develop models which can be used to sufficiently monitor less-heavily-instrumented engines.
Conclusions and Future Work

This quarter saw progress in both controlled testing and working toward effective field testing. Progress in controlled tests on the Ajax DP-115 continued this quarter. Data presented from 180-psig valve tests requires further analysis to be interpreted conclusively. Work continues toward the completion of pre-combustion-chamber testing. Although we expect field testing to be delayed until 2008, work done in the interim cooperating with gathering companies is expected to improve the quality of data that comes from the field tests. The research team believes that the preliminary work described above is necessary to achieve meaningful results from field testing.

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References


Appendix A: Data Analysis

This appendix shows the calculations used to find various quantities used in analysis of the mid-pressure fuel valve data.

(a) Average Cylinder Peak Pressure

Average peak cylinder pressure is the average of measured peak pressures over a number of cycles. $PP_{AVE} = \frac{\sum_{j=1}^{N} PP_j}{N}$, where $PP_j$ is the peak cylinder pressure for a single cycle, and $N$ is the number of cycles saved in the buffer. Each peak cylinder pressure is determined by taking the maximum pressure within a range of 45 degrees around top dead center.

$PP_{AVE}$ is calculated each second and recorded, and between these calculations, approximately five to six new values for $PP_j$ enter the buffer and the oldest few values are removed. Finally, an average cylinder peak pressure that can characterize all data in a given data set, which must be taken under constant conditions for speed, load, and other engine parameters, is found by averaging $PP_{AVE_i}$ over the number $N$ of saved averages:

$$PP_{AVE} = \frac{\sum_{i=1}^{N} PP_{AVE_i}}{N}.$$ 

Errors in each calculated quantity are determined by following the error propagation equation [10]:

$$\sigma_s^2 = \sigma_u^2 \left( \frac{\partial x}{\partial u} \right)^2 + \sigma_v^2 \left( \frac{\partial x}{\partial v} \right)^2 + \ldots$$ (1)

Either the measured standard deviation in a repeatedly measured static quantity or the stated uncertainty for the instrument is used as the error to propagate. These should be equal for a given instrument [10].

Following the error propagation equation (1), error in the average peak cylinder pressure is found to be $\delta_{PP_{AVE}} = \frac{\delta_{PP}}{\sqrt{n}}$. Here $n$ is the total number of different cycles used to find the final average because using a single data point twice, as is done in calculating average peak pressure, cannot reduce error.

(b) Average Standard Deviation of Cylinder Peak Pressure

In taking the average standard deviation of the cylinder peak pressure, a standard deviation is calculated each second for the running average of cylinder peak pressure:
\[ \sigma_i = \sqrt{\frac{\sum_{j=1}^{N} (PP_j - PP_{AVE})}{N}}. \]

These standard deviations are then averaged over \( N \), the number of data points in a set, to find

\[ \bar{\sigma} = \frac{\sum_{i=1}^{N} \sigma_i}{N}, \]

the standard deviation for a given data set.

The error in the standard deviation is calculated by taking the standard deviation of the standard deviations over the number of saved data points:

\[ \delta_{\bar{\sigma}} = \sqrt{\frac{\sum_{i=1}^{N} (\sigma_i - \bar{\sigma})^2}{N-1}}. \]

The quantity \( N-1 \) represents a loss of one degree of freedom. This is because the standard deviation uses a calculated mean rather than the actual mean of the parent distribution [10].

(c) Brake Specific Fuel Consumption

The brake specific fuel consumption expressed in BTU/hp-hr is calculated using the average of measured flow of the fuel, \( \bar{V}_f \) in SCF/hr, the average of measured torque, \( \bar{T} \) in ft-lbs, the average of measured speed, \( \bar{S} \) in rpm, and the higher heating value for fuel, \( Q_{HHV} \) in BTU/SCF, taken from a gas analysis of the fuel:

\[ BSFC = \frac{\bar{V}_f Q_{HHV}}{\bar{S} \bar{T}} \frac{5252}{5252}. \]

The error in the brake specific fuel consumption is then given as:

\[ \delta_{BSFC} = \sqrt{\left( \delta_{V_f} \right)^2 \left( \frac{BSFC}{\bar{V}_f} \right)^2 + \left( \delta_{S} \right)^2 \left( \frac{BSFC}{\bar{S}} \right)^2 + \left( \delta_{T} \right)^2 \left( \frac{BSFC}{\bar{T}} \right)^2}. \]

The error in each of the measured variables is the variable’s standard deviation, using the formula:

\[ \sigma = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1}}. \]
The bar over $x$ represents a mean calculated from $n$ experimental values of $x$.

(d) Trapped Equivalence Ratio

\[ \frac{m_f}{FA_{\text{stoich}}} \]

Trapped equivalence ratio is given by $\phi_{tr} = \frac{m_a}{FA_{\text{stoich}}}$, where $m_f$ is the mass of fuel trapped in the cylinder for one cycle, $m_a$ is the mass of the air trapped in the cylinder for one cycle, and $FA_{\text{stoich}}$ is the mass of fuel to air for stoichiometric combustion. The mass of fuel and air trapped in the cylinder are calculated from averages of measured variables, and the stoichiometric fuel-to-air ratio is calculated based on the known fuel composition.

The error in the trapped equivalence ratio is

\[ \delta_{\phi_{tr}} = \sqrt{\left( \frac{\delta_{m_f}}{m_f} \right)^2 + \left( \frac{\delta_{m_a}}{m_a} \right)^2}. \]

The trapped fuel mass is calculated by taking the average of the fuel flow divided by the average speed of the engine: $m_f = \frac{\bar{m}_f}{S}$. Its error is

\[ \delta_f = \sqrt{\left( \frac{\delta_{\bar{m}_f}}{m_f} \right)^2 + \left( \frac{\delta_S}{S} \right)^2}. \]

The trapped air mass is calculated as

\[ m_a = \frac{M_a \bar{p}_\theta V_\theta}{R_u \bar{T}_{\text{amb}} \left( \frac{\bar{p}_\theta}{\bar{p}_{\text{amb}}} \right)^{\frac{k_{\text{air}} - 1}{k_{\text{air}}}}}, \]

where $M_a$ is the molecular weight of air, $\bar{p}_\theta$ is the average absolute cylinder pressure at the angle when the exhaust port closes, $V_\theta$ is the cylinder volume at the angle when the exhaust port closes, $R_u$ is the universal gas constant, $\bar{T}_{\text{amb}}$ is the average absolute ambient temperature, $\bar{p}_{\text{amb}}$ is the average absolute ambient pressure, and $k_{\text{air}}$ is the ratio of specific heats for air. This equation comes from using the equation of states for an ideal gas, air in this case, and solving to find the mass at a certain temperature and pressure. The pressure is known because the cylinder pressure and the pressure at the exhaust port, both of which give the in-cylinder pressure when the exhaust port is still open, are known. The research team chose to use pressure at the exhaust port for this variable because it had a smaller error. The adiabatic compression equation is then substituted into the ideal gas equation to replace the in-cylinder temperature.

Although only $\bar{p}_\theta$, $\bar{T}_{\text{amb}}$, and $\bar{p}_{\text{amb}}$ are measured quantities, the calculated quantities $V_\theta$ and $k_{\text{air}}$, which is taken from a thermodynamics text [11], have errors as well. The error in trapped air mass becomes complicated:
To find the stoichiometric fuel-to-air ratio, a chemical balance for combustion, which assumes only hydrocarbons and oxygen react, is used:

\[
\begin{align*}
\text{C}_4\text{H}_y + \left(x + \frac{y}{4}\right)\text{O}_2 + 3.773\text{N}_{2,\text{ATM}} + a\text{N}_2 + b\text{CO}_2 & \rightarrow \\
x\text{CO}_2 + \frac{y}{2}\text{H}_2\text{O} + \left(x + \frac{y}{4}\right)3.773\text{N}_{2,\text{ATM}} + a\text{N}_2 + b\text{CO}_2. 
\end{align*}
\]

The variables \(x, y, a,\) and \(b\) represent the number of carbon atoms, hydrogen atoms, nitrogen molecules, and carbon dioxide molecules in a mole of fuel [1].

Then the ratio of the mass of fuel needed to the mass of the air needed is the fuel-to-air-ratio:

\[
FA_{\text{stoich}} = \frac{xM_C + yM_H + aM_{\text{N}_2} + bM_{\text{CO}_2}}{\left(x + \frac{y}{4}\right)\left(M_{\text{O}_2} + 3.773M_{\text{N}_2,\text{ATM}}\right)}. 
\]

(e) Emissions

Using basic thermodynamics, a concentration can be converted into a mass fraction,

\[
\frac{m_i}{m} = \bar{y}_i \left(\frac{M_i}{M}\right), \text{ where } m_i \text{ is the mass of a particular species, } m \text{ is the mass of the whole mixture, } \\
\bar{y}_i \text{ is the measured concentration (by number) of the species in the mixture, } M_i \text{ is the molecular weight of the species, and } M \text{ is the molecular weight of the whole mixture [11]. Dividing both masses by a unit of time gives the mass flow rate of a species: } \dot{m}_i = \dot{m}_i \bar{y}_i \left(\frac{M_i}{M}\right). \text{ Using the error propagation equation (1) the error in species flow is:}
\]
\[
\delta_{m_i} = \sqrt{\delta_{\bar{m}_i}^2 \left( \frac{\bar{m}_i}{m_i} \right)^2 + \delta_{\bar{y}_i}^2 \left( \frac{\bar{m}_i}{y_i} \right)^2 + \delta_{M_i}^2 \left( \frac{\bar{m}_i}{M_i} \right)^2}.
\]

(i) Specific Emissions

The specific emissions is the species flow divided by engine power: \( SE_i = \frac{\bar{m}_i}{ST} \). The measured quantities are the emission species concentration, needed to calculated species flow, engine speed, and engine torque. The error in each measured quality is the standard deviation in the sample of data points (equation 2). Propagating the error in the measured quantities and the calculated error in \( \bar{m}_i \) results in an error for specific emissions of:

\[
\delta_{SE} = \sqrt{\left( \delta_{m_i} \right)^2 \left( \frac{SE_i}{\bar{m}_i} \right)^2 + \left( \delta_{y_i} \right)^2 \left( \frac{SE_i}{y_i} \right)^2 + \left( \delta_{M_i} \right)^2 \left( \frac{SE_i}{M_i} \right)^2}.
\]

(ii) Total Exhaust Flow Rate

It is possible to calculate the total exhaust flow rate (the mass flow rate of the mixture) by using the combustion equation (3), when the composition of the fuel, the mass flow rate of the fuel, and \( \bar{y}_{O_2} \), the average concentration of oxygen in the exhaust, are known. Then the total exhaust flow rate, \( \bar{m}_f + \bar{m}_a \), is simply the sum of the mass flow rate of the fuel and that of the air. The air flow rate is calculated using values from the balanced chemical equation:

\[
\bar{m}_a = \frac{\bar{m}_f}{FA_{stoch}} \left[ \frac{1}{1 - 4.773\bar{y}_{O_2}} \right] \left[ \bar{y}_{O_2} \frac{(a + x + b)}{x + \frac{y}{4}} - \bar{y}_{O_2} + 1 \right].
\]

The error in the calculated mass flow of air becomes:

\[
\delta_{\bar{m}_a} = \sqrt{\delta_{\bar{m}_f}^2 \left( \frac{\bar{m}_f}{\bar{m}_f} \right)^2 + \left( \delta_{\bar{y}_{O_2}} \right)^2 \left( \frac{\bar{m}_f}{1 - 4.773\bar{y}_{O_2}} \right)^2 \left[ 4.773\bar{m}_a + \frac{a + x + b}{x + \frac{y}{4}} - 1 \right]^2}.
\]

(iii) Molecular Weights

The molecular weight of the species is 28 lbm/lbmol for CO, 30 lb/lbmol for NO, and 46 lbm/lbmol for NO2. On the other hand, the molecular weight of the exhaust must be calculated
using the various species in the exhaust and information contained in the combustion equation (3):

\[
M_t = \frac{(x + b) M_{CO_2} + aM_{N_2} + n_{O_2} M_{O_2} + 3.773 \left( \frac{\dot{m}_a}{m_f} \right) \left( x + \frac{y}{4} \right) M_{N_2, atm}}{(x + b) + a + n_{O_2} + 3.773 \left( \frac{\dot{m}_a}{m_f} \right) \left( x + \frac{y}{4} \right)}.
\]

In the calculation of molecular weight for exhaust, \( n_{O_2} \) is the number of moles of oxygen in the exhaust. This is excess oxygen. The quantity \( x + b \) is the number of moles of carbon dioxide in the exhaust and comes from the \( x \) carbon atoms in the reacting hydrocarbons as well as the \( b \) moles of non-reacting carbon dioxide. The \( a \) moles of nitrogen in the fuel also end up in the exhaust. Finally, the quantity \( 3.773 \left( \frac{\dot{m}_a}{m_f} \right) \left( x + \frac{y}{4} \right) \) gives the number of moles of atmospheric nitrogen, which actually accounts for all the gasses in the atmosphere by using \( M=28.16 \). This atomic weight for “atmospheric nitrogen” is slightly different from that of pure nitrogen [1].

The error in molecular weight of the exhaust becomes:

\[
\delta M_t = \sqrt{\delta n_{O_2}^2 \left( M_{O_2}^2 + M_t^2 \right) + \left( \delta \frac{\dot{m}_a}{m_f} + \delta \frac{\dot{m}_a}{m_f} \right)^2 + \left( 3.773 \frac{1}{m_f} \left( x + \frac{y}{4} \right) \right)^2 \left( M_{N_2, atm}^2 + M_t^2 \right)}.
\]

The number of moles of oxygen in the exhaust can be calculated using the definition of concentration: the number of moles of a species over all moles in the mixture. Solving for number of moles of oxygen gives:

\[
n_{O_2} = \frac{x + b + a + 3.773 \left( \frac{\dot{m}_a}{m_f} \right) \left( x + \frac{y}{4} \right)}{\left( 1 - \overline{y}_{O_2} \right)}.
\]

The error in the number of moles of oxygen is:

\[
\delta n_{O_2} = \sqrt{\delta n_{O_2}^2 \left( \frac{n_{O_2}}{\overline{y}_{O_2}} \right)^2 + \left( \frac{n_{O_2}}{1 - \overline{y}_{O_2}} \right)^2 + \left( \delta \frac{\dot{m}_a}{m_f} + \delta \frac{\dot{m}_a}{m_f} \right)^2 + \left( 3.773 \frac{\overline{y}_{O_2}}{1 - \overline{y}_{O_2}} \left( x + \frac{y}{4} \right) \frac{1}{m_f} \right)^2}.
\]
Appendix B: Additional Data

CO Produced at 11° BTDC

![Graph of CO produced at 11° BTDC](image)

Figure B1. At 11° BTDC, specific CO as a function of engine speed and trapped equivalence ratio.

NOx Produced at 14° BTDC

![Graph of NOx produced at 14° BTDC](image)

Figure B2. At 14° BTDC, specific NOX as a function of engine speed and trapped equivalence ratio.
Figure B3. At 14° BTDC, specific CO a function of engine speed and trapped equivalence ratio.