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A COMPARISON OF ANALYTICAL AND EXPERIMENTAL RESULTS**

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Center for Transportation Research

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ABSTRACT

Use of oxygen-enriched combustion air in diesel engines can lead to significant improvements in power density, as well as reductions in particulate emissions, but at the expense of higher NO_x emissions. Oxygen enrichment would also lead to lower ignition delays and the opportunity to burn lower grade fuels. Analytical and experimental studies are being conducted in parallel to establish the optimal combination of oxygen level and diesel fuel properties. In this paper, cylinder pressure data acquired on a single-cylinder engine are used to generate heat release rates for operation under various oxygen contents. These derived heat release rates are in turn used to improve the combustion correlation—and thus the prediction capability—of the simulation code. It is shown that simulated and measured cylinder pressures and other performance parameters are in good agreement. The improved simulation can provide sufficiently accurate predictions of trends and magnitudes to be useful in parametric studies assessing the effects of oxygen enrichment and water injection on diesel engine performance. Measured ignition delays, NO_x emissions, and particulate emissions are also compared with previously published data. The measured ignition delays are slightly lower than previously reported. Particulate emissions measured in this series of tests are significantly lower than previously reported.

INTRODUCTION

Argonne National Laboratory (ANL) has been studying the application of oxygen-enrichment technology to diesel engines, especially for industrial cogeneration systems (Assanis et al. 1990, Cole et al. 1990, Sekar et al. 1990a, and Sekar et al. 1990b). An initial assessment was based on a literature survey and a modified simulation code. The study indicated beneficial changes in engine power density, thermal efficiency, ignition delay, smoke, particulates, and other exhaust emissions. The only problem area was the increase in NO_x emissions. In order to control NO_x emissions, water was introduced into the combustion process in the form of emulsified fuel. It was also concluded that less-refined

cheaper fuel could be used with oxygen-enriched air. This fact could make the concept economically viable.

First -phase experimental work has been conducted on a single-cylinder, heavy-duty diesel engine. The experimental data have been used to fine-tune the simulation code for the oxygen-enriched diesel engine. The objective is to develop a reliable code, validated by experimental data. Such a tool would be very useful in predicting the performance of full-size cogeneration systems, using larger diesel engines, as opposed to conducting time-consuming and expensive experimentation.

This paper summarizes the original model assumptions and the modifications that were implemented in order to simulate the performance of the single-cylinder test engine with various levels of oxygen enrichment. Then, ANL experimental data are compared with simulation predictions. Also, emissions and ignition delays from the ANL data set are compared with previously published data of other investigators.

PERFORMANCE PREDICTION CODE

A turbocharged and turbocompound diesel engine computer simulation has earlier been developed by Assanis and validated against test results from a Cummins engine (Assanis and Heywood 1986). The parent code was modified at the University of Illinois in order to allow for various levels of oxygen enrichment in the intake air and for operation with water-emulsified fuels. This section briefly summarizes the main assumptions of the simulation and describes changes implemented in order to conduct our study. Additional details on the parent code can be found in Assanis and Heywood (1986).

Summary of Parent Code

In the computer simulation, the reciprocator cylinders, the intake manifold, and the various sections of the exhaust manifold are treated as a series of connected open systems.

In general, the systems are open to the transfer of mass, enthalpy, and energy in the form of work and heat. The contents of each of these systems are represented as one continuous medium by defining an average equivalence ratio and a uniform temperature and pressure at all times.

Gas properties are calculated assuming ideal gas behavior. At low temperatures (below 1000 K), the cylinder contents are treated as a homogeneous mixture of non-reacting ideal gases. At high temperatures (above 1000 K), the properties of the cylinder contents are calculated by assuming the burned gases are in equilibrium, with allowance for chemical dissociation (Martin and Heywood 1977). Provisions are incorporated in the thermodynamic property routines in order to model intake air with various levels of oxygen enrichment (i.e., with a desired N:O ratio).

The diesel four-stroke cycle is treated as a sequence of continuous processes: intake, compression, combustion (including expansion), and exhaust. Quasi-steady, adiabatic, one-dimensional flow equations are used to predict mass flows past the intake and exhaust valves. The compression process is defined to include the ignition delay period (i.e., the time interval between the start of the injection process and the ignition point). The total length of the ignition delay can either be specified or predicted using an Arrhenius expression based on the mean cylinder gas temperature and pressure during the delay period. Combustion is modeled as a uniformly distributed heat release process. The sum of two algebraic functions, one for the premixed and the other for the diffusion-controlled combustion phase is used to describe the rate of fuel burning (Watson et al. 1980). The relative weight of each combustion phase depends on the length of the ignition delay period and on the engine load and speed.

Heat transfer is included in all the engine processes. Convective heat transfer is modeled using available engine correlations based on turbulent flow in pipes. The characteristic velocity and length scales required to evaluate these correlations are obtained from a mean and turbulent kinetic energy model. Radiative heat transfer, based on the predicted flame temperature, is added during combustion. The time-dependent temperature distributions in the piston, cylinder head, liner, and manifold walls are computed using coupled, transient heat conduction models for the wall structures.

Summary of Simulation Modifications

Since the heat release correlation in the original code did not capture the effect of oxygen enrichment on combustion, an alternative option was implemented in the code to use heat release profiles based on our experimental results. First, the cylinder pressure diagrams obtained from the experiments were used to generate heat release rate diagrams as a function of oxygen content. The heat release code that was used treats the combustion chamber contents as uniformly mixed and accounts for the effects of crevice volume and in-cylinder motion. If desired, the program can also approximate the gas-to-wall heat transfer according to the Woschni correlation (Woschni 1967). More details on the heat release code are given in Bonne (1989). The experimentally derived heat release profiles were then used as inputs to the diesel computer simulation to model performance for different oxygen levels.

The original computer code could only be used with turbomachinery, and thus required specific map characteristics as an input. Simulations of naturally aspirated engines, or of single-cylinder laboratory engines with controlled intake/exhaust plenum conditions, were not possible. The new version of the code allows the option of

treating the manifolds as constant pressure and temperature plenums, in addition to the option of determining these conditions from the solution of the manifold state equations. The modified diesel simulation can now be used to model a wide variety of engine systems ranging from complex intercooled, turbocompound engines to less complicated systems, such as the naturally aspirated engine.

The original computer model required a table of measured effective valve open areas to predict mass flow rates across the valves during the gas exchange process. Since these data are often not readily available, the polydyne cam model (Assanis and Polishak 1989) was implemented in the simulation. Using this approach, the valve lift data are calculated after specifying the desired maximum lift and half-event angle. Transforming this valve lift curve into effective valve area at each crank angle involves a two-step calculation. First, a model is used to calculate the minimum area between the valve and the valve seat at each crank angle; second, the discharge coefficient for the given valve lift is calculated. The product of the minimum valve area and the discharge coefficient is equal to the effective valve area.

In order to calculate the minimum geometric valve area, the valve lift process is broken into three regimes. When lift first occurs and is still relatively small, the minimum valve area corresponds to the frustum of a right circular cone; the conical face between the valve and seat, which is perpendicular to the seat, defines the flow area. The minimum area for the next regime is still the surface of the frustum of a right circular cone, but this surface is no longer perpendicular to the valve seat. The base angle of the cone increases to 90 degrees. Finally, when the valve lift is sufficiently large, the minimum flow area is the port flow area minus the sectional area of the valve stem. Details are given in Heywood (1988).

Once the minimum valve area has been defined, the discharge coefficient is determined based on experimental data correlated to the valve area calculations. This study utilizes the discharge coefficient algorithm developed by Noyes (1980). Noyes' analytical predictions are based on experimental data for pressure ratios between 1.125 and 2.5, valve rise (valve lift divided by the valve port diameter) between 0 and 0.408, and valve seat angles between 30 and 45 degrees. A least-squares algorithm was used to determine the best correlation between pressure ratio, valve lift, and valve seat and the measured values of the discharge coefficient.

Method of Solution

When the individual sub-models of the cycle simulations are brought together to form a complete model, the result is a set of first-order ordinary differential equations. To perform predictive calculations with the cycle simulation, these equations are simultaneously integrated over the full operating cycle. Results include profiles of the state variables (such as temperature and pressure, mass flows through the valves) at specified crank angle intervals, as well as integrated performance results. The latter include power, volumetric and thermal efficiencies, gross indicated and pumping mean effective pressures, total heat loss, burn duration, and an estimated mean exhaust temperature. Heat and work transferred during each process of the cycle and the results of an overall energy balance are also provided.

EXPERIMENTAL SET-UP

Single-Cylinder Engine

A single-cylinder, four-stroke, direct-injection diesel engine was used in this series of experiments. This is a one-

cylinder version of a heavy-duty diesel engine commonly used in heavy-duty trucks and in other, off-highway applications. The major specifications of the base engine are given in Table 1. No hardware changes were made to the base engine, and the manufacturer's recommendations were followed in the set-up and operating procedures.

Table 1. Test Engine Specifications

Number of Cylinders	1
Bore x Stroke	137 mm x 165 mm
Displacement	2.44 L
Engine Speed	1800 rpm
Injection Timing	33° btdc
Compression Ratio	14.5
Peak Cylinder Pressure	11.3 MPa

Oxygen Supply System

For the purpose of the tests reported here, compressed oxygen from a bank of cylinders was used. The oxygen and the combustion air were mixed in a large tank before entering the intake manifold of the engine. A micro-fuel-cell-type (Teledyne model 326A) oxygen sensor located in the engine intake manifold was used to measure and control the intake oxygen content of the air entering the engine. Elaborate safety systems were provided to handle the compressed oxygen. The engine crank case was purged with nitrogen for added safety while running the engine. The amount of oxygen supplied from the cylinders was measured separately.

Instrumentation

For the most part, standard engine test-cell instrumentation was used for these tests. Cylinder pressure diagrams were obtained with an AVL pressure transducer, an optical encoder, and a PC-based data-acquisition system developed at the University of Illinois. NO_x and O₂ concentrations were measured in the exhaust gas stream. A conventional filter method was used to measure the particulate emissions. Two Fibertfilm TGOA20 filters were used in series to ensure high particulate collection efficiency. Details of the experimental arrangement and data collection procedures can be found in Sekar et al. (1990a, 1990b).

Test Conditions

Oxygen level of the intake air was varied from 21% to 35% by volume by mixing oxygen purchased in commercially available tanks with shop air supply. For each oxygen level, engine performance and emissions were recorded at a speed of 1800 rpm and full load. Extensive data were obtained for #2 and #4 diesel fuels and their emulsions with water. The intake and exhaust manifold pressures were maintained at 140 cm Hg abs. and 81 cm Hg abs., respectively, throughout the tests. Engine fuel rate was increased until the maximum power was reached. Engine manufacturer's recommendations were followed in the selection of these parameters (i.e., "full load" setting, boost and back pressures). This resulted in nearly constant total mass flow rate of air and oxygen. The maximum power potential at each oxygen level was reached when the exhaust oxygen level was the same as that for the base engine, or when the exhaust manifold temperature reached a generally accepted maximum value of about 630°C.

COMPARISON OF ANALYTICAL AND EXPERIMENTAL RESULTS

In this section, the measured cylinder pressure, engine power output, thermal efficiency, and intake air/O₂ mixture mass flow rates are compared to the simulation results. Only the results for non-emulsified diesel fuel are discussed here, since modeling of the effects of water injection on combustion heat release is currently being refined. The experimental ignition delays and NO_x and particulate emissions are also compared with previously published data.

Measured cylinder pressure data for the baseline case (21% oxygen content) and for the highest oxygen enrichment level (35% oxygen content) are shown in Figs. 1 and 2, respectively. These data represent smoothed profiles, derived by averaging samples of 30 engine cycles. The measured data have been processed using our heat release analysis program. Since the Woschni heat transfer correlation was developed for engines operating with base oxygen levels, there is no reason to expect it to accurately predict heat transfer under oxygen-enriched operation. For this reason, all heat release calculations are performed on a net basis (i.e., without attempting to add back a term for heat loss to the walls). As a result, the cumulative net heat release, when normalized by the fuel energy content, will not approach 100%. Nevertheless, changes in heat transfer and combustion efficiency will still appear as changes in the net heat release.

Figure 1 Comparison of measured and predicted pressure traces for baseline engine operation with 21% oxygen.

Net heat release rates for the engine operating under 21% and 35% oxygen level are shown in Figs. 3 and 4, respectively. Superposed on each of these figures is the cumulative net heat release. The injection timing is the same for both runs (i.e., 33° btdc). The effect of oxygen enrichment on heat release is noticeable. Ignition delay is shorter, so that there is almost no premixed burning. Combustion is overall more uniform with increasing oxygen content, reaches a higher peak, and ends earlier in the expansion stroke. Only 70% of the energy (on a net basis) is released with 21% oxygen, but more energy (approaching 76%) is released with 35% oxygen, indicating a more efficient combustion for the latter case.

Figure 2 Comparison of measured and predicted pressure traces for operation with 35% oxygen.

Figure 3 Net heat release rates and cumulative heat release as a function of crank angle for baseline engine operation with 21% oxygen.

Figure 4 Net heat release rates and cumulative heat release as a function of crank angle for operation with 35% oxygen.

The derived net heat release profiles were used to establish apparent rates of fuel burning; the latter were then provided as inputs to the simulation. The predicted pressure profiles for operation with 21% and 35% oxygen are compared to the measured pressure traces in Figs. 1 and 2, respectively. The same procedure was followed for the data obtained from running with 25% and 30% oxygen. Excellent comparisons of pressure levels and the rates of pressure rise are evident at all oxygen levels.

Figures 5, 6, and 7 compare predicted intake mass flow rates, brake power output, and brake thermal efficiencies against experimental data. Experimental motoring friction data for operation with 21% oxygen were used to develop a friction correlation that was used in the simulation. The variation of all three predicted performance quantities closely follows the data in both magnitude and trend. The maximum difference between the calculated and measured power and thermal efficiency is under 5%, while mass flow rates compare within 2%. The small discrepancies are attributed to possible measurement errors and to inadequacies in heat transfer and friction modeling with higher loads under oxygen enrichment. Overall, the results confirm that the simulation can provide sufficiently accurate predictions of trends and magnitudes to be useful in parametric studies assessing the effects of oxygen enrichment on engine performance. Thus, we are planning to use the model to predict performance of large-scale diesel engines with oxygen-enriched combustion air.

Figure 5 Predicted and measured intake mass flow rates as a function of oxygen concentration in the combustion air.

Figure 6 Predicted and measured brake power as a function of oxygen concentration in the combustion air.

Figure 7 Predicted and measured brake thermal efficiency as a function of oxygen concentration in the combustion air.

Figure 9 Comparison of measured NO_x emissions for various oxygen concentrations against previously published data (Iida and Sato 1988).

Emissions data obtained by ANL followed predictable trends. In general, particulate emissions decrease and NO_x emissions increase when the oxygen level is increased. Particulate data are plotted in comparison with previously published data in Fig. 8. ANL data were obtained at maximum power for each O₂ level. Since maximum power varies, it is more meaningful to plot NO_x and particulate data per kilowatt. Adequate information is not available to plot the data of Sato et al. in identical units. Hence, comparison of trends, rather than absolute values, is recommended in Figs. 8 and 9. The Argonne data do not show as large a reduction as Iida's data (Iida et al. 1986). It is possible, though, that the engine used by ANL had low particulate emissions to start with and, therefore, was not as sensitive to oxygen level.

The NO_x data in Fig. 9 agree well with previously published results (Iida and Sato 1988). Since the adiabatic flame temperatures in oxygen-rich combustion are higher, it is expected that they would result in higher NO_x levels. It is very important to control the tendency for increasing NO_x emissions if this technology is to be commercialized. Retarding fuel-injection timing and addition of water into the combustion process are two possible means to control NO_x without adverse effects on engine performance. Experimental data on water-emulsified fuel are available (Iida et al. 1986), but data on retarded injection timing effects are not yet available. As shown in Fig. 10, the ignition delay is reduced with oxygen-enriched air. Hence, retarding the injection timing is expected to reduce NO_x without any fuel consumption penalties.

Figure 8 Comparison of measured particulate emissions for various oxygen concentrations against previously published data (Iida et al. 1986).

Figure 10 Comparison of measured ignition delay for various oxygen concentrations against previously published data (Iida and Sato 1988).

CONCLUSIONS AND RECOMMENDATIONS

A computer simulation has been modified to model the performance of a diesel engine for operation with various levels of oxygen enrichment. The computer code predictions have been satisfactorily verified against experimental results. The model provides a useful tool for predicting the performance of a full-size diesel engine system using oxygen-enrichment technology. The methodology adopted here in correlating experimental data with simulation predictions should be extended to analyze results from tests with water-emulsified fuels. The measured heat release data for various oxygen and water content levels should be used to develop a more generalized heat release correlation to account for operation with oxygen enrichment and water-emulsified fuels.

Both the analysis and the test program have indicated that oxygen-enriched combustion air significantly improves the performance of a diesel engine. Higher heat release rates and an overall increase in the engine power density have been obtained. The increased combustion rate associated with oxygen enrichment may provide the opportunity for using less volatile and less expensive grades of diesel fuel. Significant increases in cylinder temperatures and pressures are also associated with oxygen enrichment.

The experimental emissions data compare well with expected trends. It has been shown that oxygen enrichment reduces the particulate and hydrocarbon emissions. Although NO_x emissions would increase (due to the higher cylinder temperatures), they could be controlled through the use of water-emulsified fuels. Overall, results are encouraging, and the technology should be tested in a full-scale application.

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