

A Thermodynamic Evaluation of the Use of Alcohol Fuels in a Spark-Ignition Engine

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ABSTRACT

Although the use of alcohol fuels in spark-ignition engines has been investigated for over 100 years, consistent and thorough thermodynamic evaluations are few. The current work examines the detail thermodynamics of the use of methanol and ethanol by an automotive, spark-ignition engine. Overall engine performance parameters, detail instantaneous quantities, and second law parameters are determined as functions of engine design and operating conditions. In addition, the results for the alcohol fuels are compared to results for isooctane. Results include indicated and brake efficiencies, heat transfer, and exhaust gas temperatures as functions of engine speed and load.

Operating conditions include constant equivalence ratio (stoichiometric), MBT spark timing, and constant burn duration. In general, the thermodynamic results are similar for the alcohol fuels and isooctane. Results for constant load (bmep = 325 kPa) resulted in a slightly more open throttle for the alcohol fuels, and hence, slightly higher thermal efficiencies for the conditions examined. In addition, the alcohol fuels resulted in slightly lower temperatures, lower nitric oxides, and less exergy destruction during the combustion process. The results are explained by detail knowledge of the relative heat transfer, pumping losses and cylinder gas temperatures.

INTRODUCTION

The use of alcohol fuels for spark-ignition engines has several advantages and disadvantages relative to the use of conventional gasoline [1–12]. The two most investigated alcohol fuels for engines appear to be methanol (CH_3OH) and ethanol ($\text{C}_2\text{H}_5\text{OH}$). Methanol is the simplest alcohol, is toxic and corrosive, and is generally

produced from coal or natural gas. Ethanol is generally not considered toxic, is soluble in water, and is biodegradable. It is generally produced from biomass (e.g., sugar, vegetables, wood), but can be produced from natural gas or oils.

Some features of alcohol fuels which are particularly attractive for spark-ignition engines include high octane numbers, relatively high heats of vaporization (potentially providing inlet charge cooling), and higher flame speeds. These features can be exploited by high-level EGR, stoichiometric, high-compression, turbocharged engines [12–13].

In the 1970s and 1980s, significant contributions were completed on the use of alcohol fuels with spark-ignition engines [1, 2]. This work has continued through the years, and further work during the 1990s and 2000s has added to the development of successful alcohol fueled engines [3–13].

With respect to evaluations of alcohol fueled, spark-ignited engines using the second law of thermodynamics, only a limited number of studies have been published. In 1992, Gallo and Milanez [14] published a study of ethanol and gasoline fueled engines which included exergy (availability) analyses. They reported that using ethanol resulted in lower destruction of exergy during the combustion process. Alasfour [15] examined the use of butanol in a single cylinder engine. He found that butanol resulted in a lower second law efficiency compared to gasoline for his operating conditions. In a study that was based on a direct injection diesel engine (not a spark-ignition engine), Rakopoulos and Kyritsis [16] presented results from their second law analysis of engine operation using methanol. They stated that that the use of me-

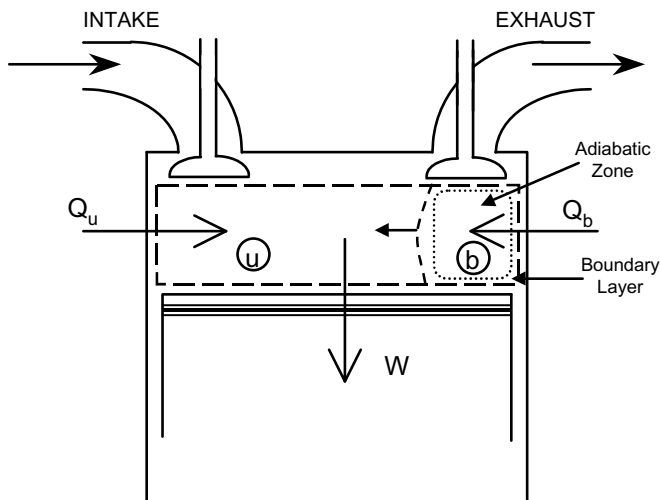


Figure 1. Schematic of the engine cylinder with the three-zone thermodynamic system denoted.

thanol resulted in lower entropy production compared to the use of n-dodecane ($n\text{-C}_{12}\text{H}_{26}$). Sezer et al. [17] found that the use of methanol and ethanol in a spark-ignited engine resulted in less entropy production. In this study, the authors' simulation was only for the valve closed portion of the cycle and they chose to examine cases with the same exergy input [17].

As described, the previous literature is somewhat limited on the use of the second law of thermodynamics to evaluate spark-ignition engines using alcohol fuels. This has provided the motivation of the current work to provide a consistent thermodynamic evaluation of the use of alcohol fuels and a comparison to iso-octane for part load and full load operation. To accomplish this objective, the study has maintained the same conditions for all fuels.

The following sections of this paper include a brief description of the cycle simulation, a synopsis of the engine and operating conditions, and a presentation of the results. The results will include overall and detail engine and thermodynamic parameters, and results for nitric oxide production. Finally, this paper will end with a brief summary and conclusions.

ENGINE CYCLE SIMULATION DESCRIPTION

The cycle simulation used in this work has been described in detail elsewhere [18–23], and is summarized in appendix A. This simulation is largely based on thermodynamic formulations, and is a complete representation of the four-stroke cycle including the intake, compression, combustion, expansion and exhaust processes. The simulation uses detailed thermodynamic gas properties including equilibrium compositions for the burned gases [24]. The cylinder heat transfer is adopted from the correlation by Woschni [25], and the combustion process is based on a mass fraction burn relation from Wiebe [26]. The Wiebe function is based on a two-parameter expression; and for this study, these parameters

Table 1. Engine Specifications

Item	Current
Number of cylinders	8
Bore (mm)	101.6
Stroke (mm)	88.4
Crank Rad/Con Rod	0.305
Compression Ratio	8.1:1
Inlet Valves:	
Diameter (mm)	50.8
Max Lift (mm)	10.0
Opens ($^{\circ}\text{CA aTDC}$)	357
Closes ($^{\circ}\text{CA aTDC}$)	-136
Exhaust Valves:	
Diameter (mm)	39.6
Max Lift (mm)	10.0
Opens ($^{\circ}\text{CA aTDC}$)	116
Closes ($^{\circ}\text{CA aTDC}$)	371
Valve Overlap (degrees)	14 $^{\circ}$

were: $m = 2.0$ and $a = 5.0$. These parameters have been matched to experimental data in other studies as explained in [23].

The intake and exhaust processes are based on equations for one-dimensional, quasi-steady flow that are corrected by an empirical discharge coefficient. The intake and exhaust manifolds are assumed to be at constant pressures. The instantaneous valve lift is approximated with a sinusoidal shape based on valve timings and maximum valve lift [27].

The combustion model uses three zones which provides a better representation of the temperatures during the combustion process. The effects of using multiple zones are described elsewhere [18]. Figure 1 shows a schematic of the engine cylinder and the three zones during combustion. First, the formulation is developed for an unburned and burned zone. Then, the burned zone is expanded into an adiabatic zone and a boundary layer. The total heat transfer is divided in an appropriate fashion between the unburned and burned zone. The heat transfer to the burned zone is assigned in total to the boundary zone.

The engine friction includes the mechanical friction (rubbing friction and work for auxiliaries such as pumps) and the pumping friction. The friction was computed using algorithms as supplied from the literature [28].

The second law analysis may be completed once the final cycle thermodynamics are determined. The details of this portion of the simulation are also included in appendix A. To determine values for the exergy, the entropy is needed which may be found from the other thermodynamic properties. The increase of entropy due to irreversibilities may be obtained from an entropy balance which accounts for entropy flow into and out of the system and any heat transfer.

The exergy may then be determined based on the entropy and other thermodynamic properties. The exergy destroyed by irreversibilities is obtained from an exergy balance. As an internal consistency check, the exergy destroyed also may be found from the entropy production during the combustion process [18].

ENGINE, FUELS AND OPERATING SPECIFICATIONS

The selected engine for these studies was an automotive V-8 configuration with a compression ratio of 8.1:1, and with a bore and stroke of 101.6 and 88.4 mm, respectively (table 1 lists these and other engine specifications). This engine is the same as has been used in a number of previous studies [18–23] where other details may be found.

Table 2 is a list of the properties of the alcohol fuels and isooctane [29]. Included in the list are the molecular formula, the stoichiometric mass air-fuel ratio, the lower heating value (LHV), the heating value for a stoichiometric mixture, the fuel exergy, and the enthalpy of vaporization. Although the heating values (on a per fuel mass basis) of the alcohol fuels are about one half of the value for isooctane, the heating values of the stoichiometric mixtures are approximately the same. This results, for example, in similar adiabatic flame temperatures for the three fuels [22]. The fuel exergy values are slightly higher than the lower heating values.

An important feature of the alcohol fuels is their relatively high energy of vaporization. Some of the consequences of this feature include cold starting issues, and the potential for temperature decreases of the inlet charge. This is examined below. For most of these computations, however, the fuel was assumed completely vaporized and uniformly mixed with the incoming air.

RESULTS AND DISCUSSION

The results of this study are presented in three sections: results for the base case, results as functions of engine speed, and results as functions of engine load. Additional results are presented in appendix B.

BASE CASE RESULTS – These first results will include results of cylinder pressure and temperatures, effects of

Table 3. Engine and Fuel Input Parameters
(Base Case: isooctane, bmep = 325 kPa, $r = 8.1$,
EGR = 0%, MBT timing)

Item	Value
Displaced Volume (dm^3)	5.733
Equivalence Ratio	1.0
Frictional mep (kPa)	74.8
Inlet Pressure (kPa)	49.9
Exhaust Pressure (kPa)	104.4
Engine Speed (rpm)	2000
Start of Combustion ($^\circ\text{bTDC}$)	21.5
Combustion Duration ($^\circ\text{CA}$) (defined as 0 – 100%)	60
Inlet (air-fuel) Temperature (K)	319.4
Cylinder Wall, Piston and Head Temperature (K)	450

inlet charge temperature, and second law parameters. These results are for the 2000 rpm, and either part load (bmep = 325 kPa) or wide open throttle conditions. Table 3 lists some of the input engine and fuel parameters. As described in table 3, the inside cylinder surfaces (cylinder wall, piston top, valves, and bottom of cylinder head) were assumed to have a uniform temperature of 450 K. The mechanical friction mean effective pressure was 74.8 kPa for this set of conditions.

Both the cylinder pressures and the overall, one-zone average cylinder gas temperatures were similar for the three fuels for the base case operating conditions [22]. This was at least partially due to the constant speed and load operating conditions. As shown next, the throttle required adjustment for the three fuels to obtain the constant load. For these base case conditions, the maximum cylinder pressure for the methanol case was about 55 kPa higher than for the isooctane case with ethanol case in between. The maximum gas temperature for the isooctane case was about a 41 K higher than the methanol case with ethanol in between.

As mentioned above, an important aspect of the use of alcohol fuels is the fuel vaporization in the intake system for port injected engines. This is a complex process that depends on many design and operational details such as the intake geometry, coolant flow conditions, transit times, injection characteristics and engine operating conditions. In general, inlet charge temperature decreases due to the fuel vaporization are in the range of a few degrees to about 25 K [30]. Rather than attempt a detail evaluation, this study will illustrate the general nature of the effect of this inlet charge temperature decrease on engine performance and nitric oxide.

Figure 2 shows the brake thermal efficiency as functions of the decrease of the inlet charge temperature for the part load base case conditions for the three fuels. The alcohol fuels have a slightly higher brake efficiency compared to the isooctane case. This is explored further in the results below.

Table 2. Properties of the Fuels [13]

Fuel Vapor	Formula	AF _{stoich}	LHV (MJ/kg _{fuel})
Isooctane	C ₈ H ₁₈	15.07	44.4
Methanol	CH ₄ O	6.45	20.0
Ethanol	C ₂ H ₆ O	8.97	26.9
Fuel Vapor	HV for stoich mixture (MJ/kg _{mix})	Fuel Exergy (MJ/kg _{fuel})	h _{fg} (kJ/kg)
Isooctane	2.76	45.5	308
Methanol	2.68	21.1	1103
Ethanol	2.70	28.4	840

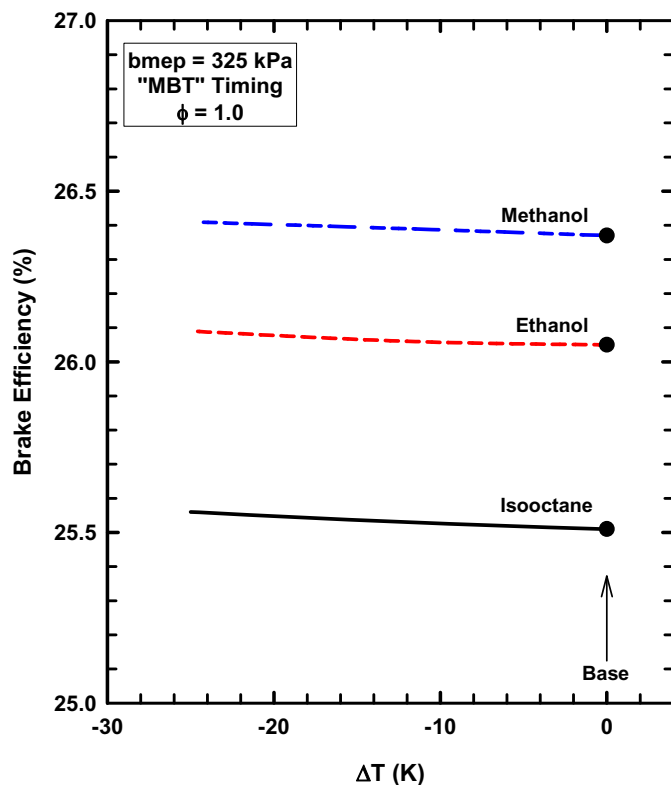


Figure 2. Brake thermal efficiency as functions of the inlet charge temperature decrease due to vaporization for the three fuels for the *part load* operating conditions.

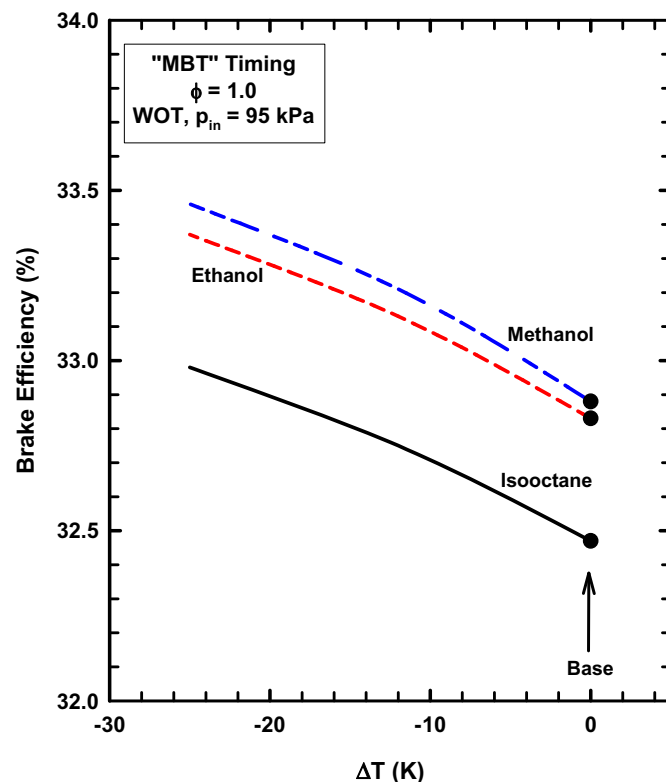


Figure 4. Brake thermal efficiency as functions of the inlet charge temperature decrease due to vaporization for the three fuels for the *WOT* operating conditions.

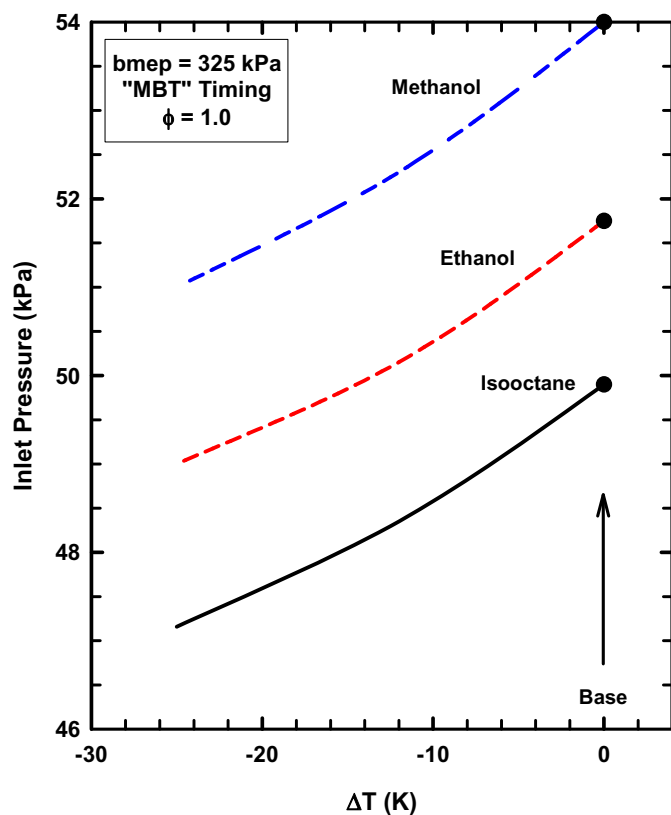


Figure 3. Required inlet pressure (to attain the constant load) as functions of the inlet charge temperature decrease due to fuel vaporization for the three fuels for the *part load* operating conditions.

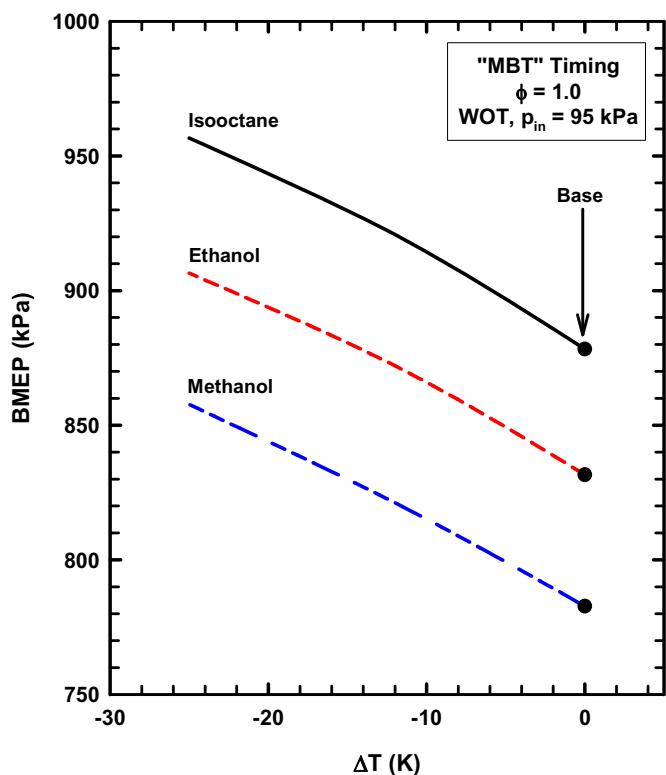


Figure 5. Brake mean effective pressure as functions of the inlet charge temperature decrease due to vaporization for the three fuels for the *WOT* operating conditions.

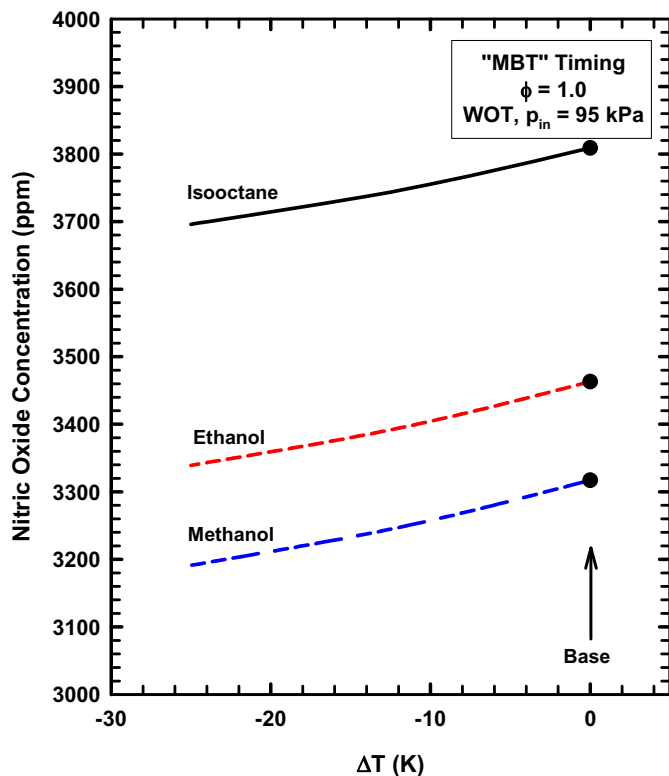


Figure 6. Nitric oxide concentrations as functions of the inlet charge temperature decrease due to vaporization for the three fuels for the *WOT* operating conditions.

The effect of the inlet charge temperature decrease is negligible for these conditions. Since these results are for constant load (bmep), the inlet pressure was adjusted as needed to attain the constant load. Figure 3 shows the inlet pressure required as functions of the decrease of the inlet charge temperature decrease for the part load base case conditions for the three fuels. The inlet pressure needed to decrease as the temperature of the inlet charge decreased due to fuel vaporization. In other words, although the temperature decrease of the inlet charge may have been favorable, this was somewhat negated by the needed inlet pressure decrease to attain the constant load.

The above may suggest that the results would be different for wide open throttle (WOT) conditions. For these considerations, the inlet manifold pressure was assumed constant at 95 kPa. Figure 4 shows brake thermal efficiency as functions of the decrease of the inlet charge temperature decrease for the WOT conditions for the three fuels. The brake thermal efficiency increases (almost 0.5% for a temperature decrease of 25 K) as the temperature decrease increases.

For WOT conditions, the other results relate to the specific maximum power and the nitric oxide emissions. Figure 5 shows the bmep as functions of the inlet charge temperature decrease for the WOT conditions for the three fuels. As the inlet charge temperature decreases, the bmep increases. For a 25 K decrease of the inlet charge temperature, for isooctane (and similar for the two alcohol fuels), the bmep increases about 8.5%.

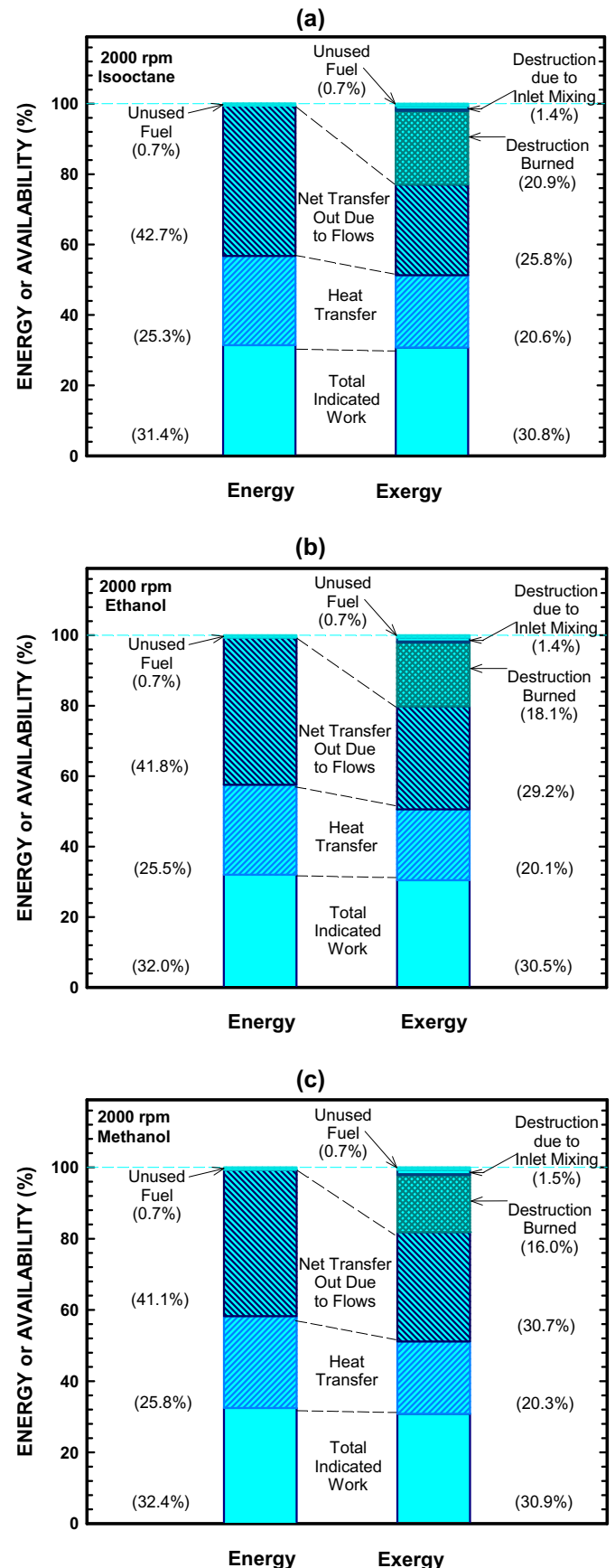


Figure 7. Percentage of fuel energy and exergy (availability) for 2000 rpm for the three fuels for the base case operating conditions.

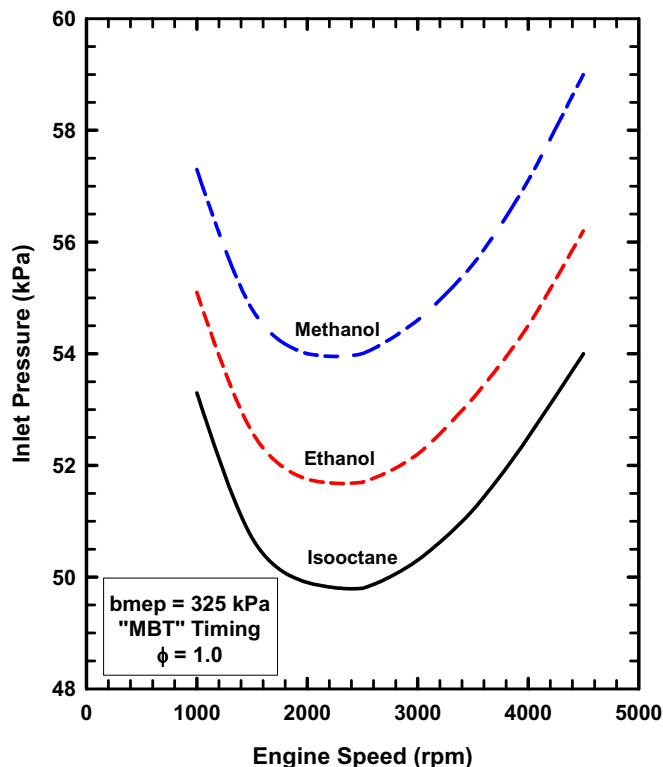


Figure 8. Inlet pressure as functions of engine speed for the three fuels for the base case operating conditions.

For WOT conditions, figure 6 shows the nitric oxide concentrations as functions of the inlet charge temperature decrease for the WOT conditions for the three fuels. As the inlet charge temperature decreases, the nitric oxide concentrations decrease slightly. For isooctane for a 25 K inlet charge temperature decrease, the nitric oxide concentration decreases about 2.9%.

As mentioned above, the remaining computations are completed for a constant inlet charge temperature (319.3 K).

Figure 7 includes three bar graphs which illustrate the percentage distribution of the energy and exergy values for the three fuels for the part load base case operating conditions at 2000 rpm. For all these figures, the left-hand bar is for the first law (energy) analyses, and the right-hand bar is for the second law (exergy) analyses. First, with respect to the net indicated work, the values using energy units are the same since the indicated work is 100% available energy. The percentages, however, are slightly different due to the slightly higher exergy of the fuel relative to its energy value (see table 2).

For the heat loss, for all fuels, about 25% of the fuel energy is transferred, but only about 20% of the fuel exergy. Similarly, for the net flow out, about 42% of the energy is expelled, but only about 25% to 31% (depending on the fuel) of the exergy is expelled. The next two categories apply only to the exergy accounting, and not to the first law (energy) aspect. These two categories quantify the exergy destruction due to combustion and

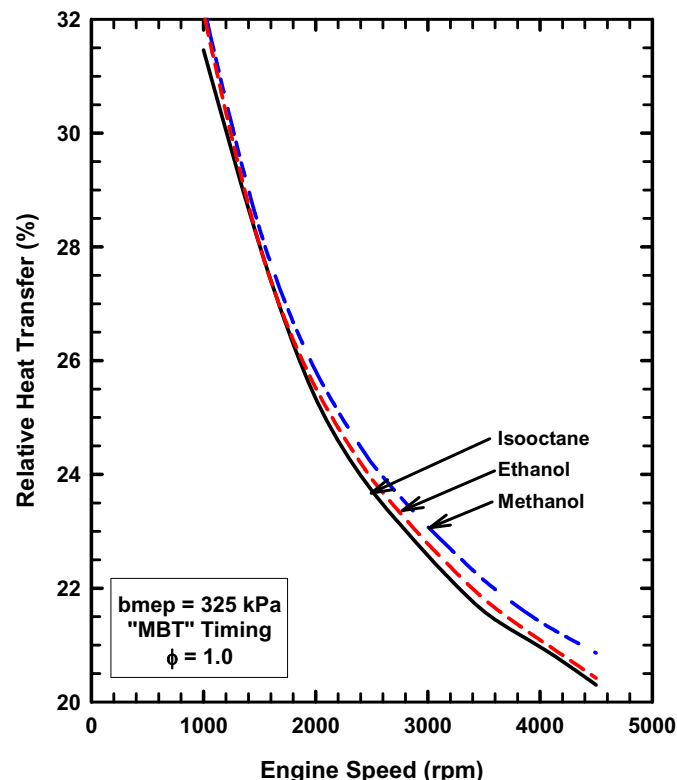


Figure 9 Relative heat transfer (as percentage of input energy) as functions of engine speed for the three fuels for the base case operating conditions.

inlet mixing. For the inlet mixing, the amount destroyed was small and about the same for the three fuels.

The combustion process is responsible for about 21%, 18% and 16% of the exergy destruction for isooctane, ethanol and methanol, respectively. In general, this is due to the highly irreversible nature of the combustion process. The mechanical irreversibility due to friction during the expansion stroke is reported separately. The alcohol fuels result in slightly lower exergy destruction due their simpler molecular structure. The slightly higher exhaust exergy for the alcohol fuels is at least partly due to this preservation of the exergy. The destruction of exergy during the combustion process is further evaluated below as functions of engine speed and load. These results are consistent with the previously discussed references [14–17].

EFFECTS OF ENGINE SPEED – Figure 8 shows the required inlet manifold pressures as functions of engine speed for the three fuels for the base case operating conditions. In general, higher inlet pressures (less throttle) are needed for the alcohol fuels to achieve the constant bmeep. This higher inlet pressure compensates for the higher fraction of fuel vapor for the alcohol fuels which displaces air and lowers the fuel energy density. The shape of these curves is a net result of the brake specific fuel consumption (or brake thermal efficiency) – as is shown below.