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Improved Engine Design Concepts Using the Second Law of Thermodynamics

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Executive Summary

This project was aimed at developing and using numerical tools which incorporate the second law of thermodynamics to better understand engine operation and particularly the combustion process. A major activity of this project was the continual enhancement and use of an existing engine cycle simulation to investigate a wide range of engine parameters and concepts. The major motivation of these investigations was to improve engine efficiency. These improvements were examined from both the first law and second law perspective.

One of the most important aspects of this work was the identification of the combustion irreversibilities as functions of engine design and operating parameters. The combustion irreversibility may be quantified in a number of ways but one especially useful way is by determining the destruction of exergy (availability) during the combustion process. This destruction is the penalty due to converting the fuel exergy to thermal energy for producing work.

The engine cycle simulation was used to examine the performance of an automotive (5.7 liter), V-8 spark-ignition engine. A base case was defined for operation at 1400 rpm, stoichiometric, MBT spark timing with a bmep of 325 kPa. For this condition, the destruction of exergy during the combustion process was 21.0%. Variations of many engine parameters (including speed, load, and spark timing) did not alter the level of destruction very much (with these variations, the exergy destruction was within the range of 20.5–21.5%). Also, the use of turbocharging or the use of an over-expanded engine design did not significantly change the exergy destruction. The exergy destruction during combustion was most affected by increased inlet oxygen concentration (which reduced the destruction due to the higher combustion temperatures) and by the use of cooled EGR (which increased the destruction).

This work has demonstrated that, in general, the exergy destruction for conventional engines is fairly constant (~21%) for a range of operating and design parameters. Further, to achieve high efficiency engines requires that the exergy be *managed* and not necessarily reduced. The overall thermodynamics is the final discriminator regarding high efficiency engines.

INTRODUCTION

This project was aimed at developing and using numerical tools which incorporate the second law of thermodynamics to better understand engine operation and particularly the combustion process. With these tools, engine concepts for higher efficiency were examined. The project included investigations of both simple systems and complete engine systems.

This project has resulted in numerous publications, presentations and theses. Appendix A is a list of these items.

The major effort of this work involved the continual enhancement and use of an engine cycle simulation and this work is highlighted in this final report. The work involving the simple systems has been documented in several publications and theses. Appendix B includes a copy of one of these publications. The work completed with the simple systems was valuable for understanding the combustion irreversibilities in more detail, but to help focus this final report, these results will not be reviewed here. Therefore, the remaining portions of this report will concern only the engine simulations.

Engine cycle simulations have been developed and used to study a variety of features and issues relative to internal-combustion engines for almost a half century. In the beginning, engine cycle simulations were fairly elementary, and were limited by both computing capabilities, and a lack of knowledge concerning key sub-models. In time, these simulations have become more complete and useful. Today, these engine cycle simulations are sophisticated, complex computer programs that provide both global engine performance parameters as well as detail information. Many of these simulations contain advanced and detailed sub-models for the fluid mechanics, heat transfer, friction, combustion and chemical kinetics.

The more advanced simulations include calculations in three-dimensions. Some of these simulations are grouped in the general category of Computational Fluid Dynamics (CFD) (Mattavi and Amann, 1980; Ramos, 1989). These CFD simulations are outside the scope of the current work.

The focus of the current work is the development and use of zero-dimensional, thermodynamic engine simulations. Thermodynamic engine simulations contain a

number of important features. Although thermodynamic simulations generally provide no detail spatial information, they do provide time (or crank-angle) varying quantities such as cylinder gas pressure and temperature, heat release, heat loss, intake and exhaust flow rates, and cylinder mass. In addition, these simulations are typically more practical than the multi-dimensional simulations for extensive parametric studies and other related investigations.

The objective of the current work was to expand an existing simulation to include multiple zones for the combustion process. Once the simulation was formulated, the simulation was validated by comparison to existing work, and then used to evaluate a number of engine parameters and thermodynamic properties.

The following sections of this report include a summary of background information, a description of the model development, a synopsis of the engine and operating conditions, and a presentation of the results. The description of the model development will include sections on the one-zone formulation, the multiple zone formulations, the items necessary for solving the governing equations, the thermodynamic properties, and the solution procedures. The results will include overall and detail engine and thermodynamic parameters. In addition, the results will include comparisons to previous related work which will serve as a form of verification. Finally, this report will end with a brief summary and conclusions.

BACKGROUND

As mentioned above, the development and use of thermodynamic engine cycle simulations have been reported since the early 1960s. The original simulations were based on one-zone and two-zone formulations, and then these type of simulations were extended to include three or more zones. Patterson and van Wylen (1964) reported one of the first thermodynamic simulations that included unburned and burned zones, progressive combustion, heat transfer, and flame propagation for uniform (homogeneous) charge engines. Their simulation did not, however, include flow rates, heat transfer from the unburned zone, and other features. Nevertheless, in many ways this simulation was a signal achievement, and the start of a long history of the development and use of thermodynamic engine simulations. Interestingly, this

work also included one of the first presentations of the results of an exergy (availability) analysis. A summary of investigations on availability analysis for reciprocating engines is available from Caton (2000).

A study by Heywood *et al.* (1979) described one of the first simulations using multiple zones for the combustion process. For their formulation, the burned zone was divided into an adiabatic core and a boundary layer zone in addition to the unburned zone. The details of this formulation and their results are summarized in subsequent portions of the current report.

Blumberg *et al.* (1980) published a review of these types of cycle simulations, and described the use of multiple zone simulations. In particular, they noted that the use of a boundary layer zone allows a better representation of the heat loss which is known to be confined largely to the region near the walls. James (1982) also commented on the importance of multiple zones for predicting nitric oxide emissions.

Raine *et al.* (1995) have published results from a cycle simulation using multiple zones for the burned gas. They were able to show that importance of multiple zones especially for the computation of nitric oxides. This work did not include the specific use of a boundary layer and did not include flows.

Although a complete citation of all investigations in this area is beyond the scope of the current work, a few examples of some additional work will be mentioned. Other work is available on the use of multiple zones to describe the combustion process (*e.g.*, Chomiak *et al.*, 1991). Some of this other work provides additional features such as in-cylinder flow and turbulence, detailed models of heat transfer, and flame propagation (*e.g.*, Wahiduzzaman *et al.*, 1993). Some of this other work has applied the multiple zone approach to heat release analysis (Egnell, 1998).

As described above, the use of multiple zones to describe the combustion process has a number of advantages. Because of these advantages, the objectives of the current work include the development and use of such a simulation. Two specific goals were (1) to emphasize a high level of accuracy in the energy accounting, and (2) to provide detail descriptions of the thermodynamics for typical spark ignition engine cycles.

MODEL DESCRIPTION

Many of the features of the overall cycle simulation have been well documented elsewhere (see *e.g.*, Caton, 2002). The major assumptions and approximations used in the development include the following:

- (1) the thermodynamic system is the cylinder contents (see figure 1).
- (2) the engine is in steady-state such that the thermodynamic state at the beginning of each cycle (two crank-shaft revolutions) is equivalent to the state at the end of the cycle.
- (3) for the compression, expansion and exhaust processes, the cylinder contents are spatially homogeneous and occupy one zone.
- (4) for the intake process, two zones (each spatially homogeneous) are used. One zone consists of the fresh charge and the other zone consists of the residual gases.
- (5) for the combustion processes, three zones (each spatially homogeneous) are used. The three zones are: the unburned zone, the adiabatic core burned zone, and the boundary layer burned zone. The adiabatic core and boundary layer zones together comprise the burned zone.
- (6) the thermodynamic properties (including pressure and temperature) vary only with time (crank angle) and are spatially uniform in each zone.
- (7) the instantaneous composition is obtained from generally accepted algorithms (Heywood, 1988) and the species obey the ideal gas equation of state.
- (8) the instantaneous thermodynamic properties are computed from established formulations (Heywood, 1988) based on the appropriate compositions.
- (9) the flow rates are determined from quasi-steady, one-dimensional flow equations, and the intake and exhaust manifolds are infinite plenums containing gases at constant temperature and pressure.
- (10) the fuel is completely vaporized and mixed with the incoming air.
- (11) the combustion efficiency was 100% (*i.e.*, no unburnt fuel¹).
- (12) the blow-by was zero.

The majority of the above assumptions and approximations have been validated and used in a number of previous simulations (see *e.g.*, Caton, 2002). Additional features have been added during the course of this work and are described below.

¹The use of the Wiebe function for the mass fraction burned (described below) results in a small amount of unburned fuel at the end of the combustion period. For example, for values of the constants $a = 5.0$ and $m = 2.2$, this small amount is 0.67% of the original fuel mass.

The current form of the simulation is limited to in-cylinder processes. For simplicity, the combustion chamber was assumed to be a cylindrical shape. For this work, all cylinders of a multiple-cylinder engine are assumed to be identical, to possess the same thermodynamics, and to operate with identical conditions. This means, therefore, that overall results for a multiple-cylinder engine are obtained by multiplying the results from the single-cylinder analysis by the number of cylinders.

The primary feature used in the development of this cycle simulation is the first law of thermodynamics which is utilized to derive expressions for the time (crank-angle) derivative of the pressure, gas temperatures, and volumes in terms of engine design variables, operating conditions, and submodel parameters.

One-Zone Formulation: A one-zone formulation is appropriate for the compression, late expansion, and exhaust processes. The first law of thermodynamics for the one-zone formulation for this system is

$$\frac{dE}{dt} = \frac{dQ}{dt} - \frac{dW}{dt} + \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} \quad (1)$$

As described elsewhere (Caton, 1998), this equation may be used to find an explicit relation for the derivative of the overall average cylinder gas temperature:

$$\dot{T}_{avg} = \frac{G(1+P_1)}{mC_v(1+P_2)} \quad (2)$$

where,

$$G = (\dot{Q} - p\dot{V} + \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} - u\dot{m}) \quad (3)$$

$$P_1 = \alpha_1/G \text{ and } P_2 = \alpha_2/C_v \quad (4)$$

$$\alpha_1 = m \left\{ \frac{\partial u}{\partial \phi} \dot{\phi} + \frac{\partial u}{\partial p} \frac{\partial p}{\partial \phi} \left(-mT_{avg} \frac{\partial R}{\partial \phi} \dot{\phi} - \dot{m}RT_{avg} + p\dot{V} \right) \right\} \quad (5)$$

$$\alpha_2 = \frac{\partial u}{\partial p} \frac{\partial p}{\partial \phi} p \left(\frac{1}{T_{avg}} + \frac{1}{R} \frac{\partial R}{\partial T} \right) \quad (6)$$

$$\beta = \left(1 - \frac{p}{R} \frac{\partial R}{\partial p} \right) \quad (7)$$

Eq. 2 may be integrated to find the average gas temperature. The corresponding cylinder pressure is then found from the ideal gas equation.

For the inlet process, an expression similar to eq. 2 is needed, but this expression must account for the two different substances that exist during intake (fresh charge and residual gases). This expression is somewhat more complicated, but in general, has the same form. For this case, a mass rate of mixing is required, and for the inlet process, this is given by the inlet flow rate. Complete details for this case are provided by Caton (1998).

Two-Zone Formulation: For the combustion process, multiple zones are used. First, the formulation is presented for two zones: an unburned zone and a burned zone. Then, the formulation is extended such that the burned zone may be divided into an adiabatic core zone and a boundary layer zone. Figure 1 is a schematic of the two zones. As shown, the combustion gases are divided into a burned and an unburned portion. The total heat transfer is divided into portions for each zone. The burned zone entrains mass from the unburned zone as the flame front proceeds.

The energy equations for the two zones are

$$\frac{d(mu)_b}{d\theta} = \dot{Q}_b - p\dot{V}_b + \dot{m}_b h_u \quad (8)$$

$$\frac{d(mu)_u}{d\theta} = \dot{Q}_u - p\dot{V}_u + \dot{m}_u h_u \quad (9)$$

Derivatives for the two temperatures, the pressure, and the two volumes may be derived. Complete details are available elsewhere (Caton, 2001). The result of the derivation is the following five ordinary differential equations:

$$\begin{aligned} \dot{T}_b &= \frac{\dot{Q}_b - p\dot{V}_b + \dot{m}_b(h_u - u_b) - m_b(\partial u_b/\partial p)\dot{p} - m_b(\partial u_b/\partial \phi)\dot{\phi}}{m_b C_{v,b}} \\ \dot{T}_u &= \frac{\dot{Q}_u - p\dot{V}_u + \dot{m}_u R_u T_u}{C_{v,u} m_u} \\ \dot{V}_b &= V_b \left(\frac{\dot{T}_b}{T_b} + \frac{\dot{m}_b}{m_b} + \frac{\dot{R}_b}{R_b} - \frac{\dot{p}}{p} \right) \\ \dot{V}_u &= \dot{V} - \dot{V}_b \\ \dot{p} &= \frac{(m_b R_b \dot{T}_b + m_b((\partial R_b/\partial T)\dot{T}_b + (\partial R_b/\partial \phi)\dot{\phi})T_b)}{V \left(1 - \frac{m_b(\partial R_b/\partial p)T_b}{V} \right)} \\ &\quad + \frac{\dot{m}_b(T_b R_b - T_u R_u) + m_u R_u \dot{T}_u - p\dot{V}}{V \left(1 - \frac{m_b(\partial R_b/\partial p)T_b}{V} \right)} \end{aligned} \quad (10)$$

Figure 1. Schematic of the two-zone thermodynamic system.

The solution of the above set of ordinary differential equations (ODEs) is described below. Once the unburned and burned temperatures (T_u and T_b , respectively) are known, an overall, average cylinder gas temperature may be determined from the overall energy balance:

$$m_{cyl}u_{avg} = m_u u_u + m_b u_b \quad (11)$$

Since the overall cylinder internal energy (u_{avg}) is not known, an estimate is obtained for the overall cylinder temperature:

$$T_{avg}^{est} = \frac{m_u C_{v,u} T_u - m_b C_{v,b} T_b}{m_{cyl} C_{v,cyl}} \quad (12)$$

Using the ideal gas equation, the corresponding estimated cylinder pressure, p^{est} , may be found. Now the internal energy may be obtained,

$$u_{avg}^{est} = \text{function}(T_{avg}^{est}, p^{est}, \dots) \quad (13)$$

The overall cylinder temperature (and pressure) are adjusted until the energy balance (eq. 11) is satisfied.

Three-Zone Formulation: The next step is to divide the burned zone into the boundary layer and adiabatic core zones. Figure 2 is a schematic of the boundary layer and adiabatic zones. Initially, the boundary layer has zero mass, and the adiabatic core is equal to the burned mass. As shown, the boundary layer increases in mass by entraining mass from the adiabatic core. The rate of mass entrainment of the boundary layer is dictated by the thermodynamics and temperature relations (described be-

Figure 2. Schematic of the adiabatic and boundary layer zones.

low). All the burned gas heat transfer is assigned to the boundary layer.

For these additional two zones, the formulation of the energy equation is similar to the above for the overall system. The first law, then, for the adiabatic and boundary layer zones, respectively, are:

$$\frac{d(mu)_a}{d\theta} = -p\dot{V}_a + \dot{m}_b h_u - \dot{m}_{bl} h_a \quad (14)$$

$$\frac{d(mu)_{bl}}{d\theta} = \dot{Q}_b - p\dot{V}_{bl} + \dot{m}_{bl} h_a \quad (15)$$

The growth of the boundary layer is dictated by the mass and energy conservation relations for the burned zone. A choice at this point is how the average boundary layer temperature is defined. One classical definition for the average boundary layer temperature is based on a logarithmic relation of the wall temperature and the adiabatic zone temperature:

$$T_{bl} = \frac{T_a - T_{wall}}{\ln(T_a / T_{wall})} \quad (16)$$

In addition, the derivative of this expression may be derived,

$$\dot{T}_{bl} = \left[\frac{1}{\ln(T_a / T_{wall})} - \frac{1 - T_{wall} / T_a}{(\ln(T_a / T_{wall}))^2} \right] \dot{T}_a \quad (17)$$

To summarize, the new unknowns for the boundary layer and adiabatic core zones are T_a , T_{bl} , V_a , V_{bl} , m_a and m_{bl} . A number of different sets of differential equations may be formulated for these variables. Because these differential equations are highly nonlinear and exhibit complex interrelations, not all combinations of the

above equations were successful. After extensive trials, the following six (6) ordinary differential equations for these variables were found to be the most robust in terms of obtaining stable solutions:

$$\begin{aligned}
\dot{T}_a &= \frac{-p\dot{V}_a + \dot{m}_b(h_u - u_a) - \dot{m}_{bl}(R_a T_a)}{C_{v,a}m_a} \\
&\quad + \frac{-m_a(\partial u_a / \partial p)\dot{p} - m_a(\partial u_a / \partial \phi)\dot{\phi}}{C_{v,a}m_a} \\
\dot{T}_{bl} &= \left[\frac{1}{\ln(T_a/T_{wall})} - \frac{1 - T_{wall}/T_a}{(\ln(T_a/T_{wall}))^2} \right] \dot{T}_a \\
\dot{V}_{bl} &= V_{bl} \left(\frac{\dot{m}_{bl}}{m_{bl}} + \frac{\dot{R}_{bl}}{R_{bl}} + \frac{\dot{T}_{bl}}{T_{bl}} - \frac{\dot{p}}{p} \right) \\
\dot{V}_a &= \dot{V}_b - \dot{V}_{bl} \\
\dot{m}_{bl} &= \frac{1}{u_{bl} - h_a} (\dot{Q}_b - p\dot{V}_{bl} \\
&\quad - m_{bl}((\partial u_{bl} / \partial p)\dot{p} - m_{bl}(\partial u_{bl} / \partial \phi)\dot{\phi} - \dot{T}_{bl}C_{v,bl})) \\
\dot{m}_a &= \dot{m}_b - \dot{m}_{bl}
\end{aligned} \tag{18}$$

Complete details are available elsewhere (Caton, 2001).

Items for the Gas Temperature Derivative Equation:

To solve the above governing differential equations (eq. 2, 10 and 18), several items are needed. These items include the thermodynamic properties, the mass fraction burned, the convective heat transfer, and the mass flow rates. These items are described next.

Thermodynamic Properties: The thermodynamic properties needed for solving the first law include the instantaneous specific internal energy, specific enthalpy, specific gas constant, molecular mass, and six (6) property derivatives (Caton, 1998; Caton, 1999a). All the properties are needed as a function of time (crank angle) for the cylinder contents for the three zones, and for any matter entering the cylinder.

Depending on the specific processes during a cycle, the thermodynamic properties may be for different mixtures of air, fuel vapor, and combustion products. The concentrations of the combustion products may be “frozen” for the lower temperatures, or these concentrations may be based on an instantaneous determination of chemical equilibrium (see e.g., Olikara and Borman, 1975) for higher temperatures. For this work, for temperatures greater than a “switch” temperature (T_{switch}), the equilibrium concentrations were used. Complete descriptions of the algorithms used for determining the composi-

tions are presented in a number of references (e.g., Heywood, 1988; Caton, 1998).

Once the composition is known, the individual thermodynamic properties may be determined. The properties of each species in the mixture are first determined for the given temperature and pressure by the use of polynomial curve fits (Heywood, 1988) to the thermodynamic data. The overall mixture properties are then determined by suitable expressions.

Mass Fraction Burned: The mass fraction of fuel (or fuel mixture) burned (x_b) may be determined from a first-law analysis of the measured cylinder pressure (Heywood, 1988). The result of this analysis is almost always an “S” shape type curve. The mass fraction burned is defined as

$$x_b = \frac{(m_f)_{burned}}{(m_f)_{total}} \tag{19}$$

The current work has used the Wiebe function (Wiebe, 1970) to represent the mass fraction burn

$$x_b = 1 - \exp\{-ay^{m+1}\} \tag{20}$$

where y is a non-dimensional time variable,

$$y = \frac{\theta - \theta_o}{\theta_b} \tag{21}$$

and where “ a ” and “ m ” are parameters that are selected to provide a match with experimental information. The values that provide a good match with the data depend on complex functions of the turbulence, chemistry, fuel, equivalence ratio, chamber geometry, and a number of other features. The values used here are based on the work of Heywood *et al.* (1979):

$$a = 5.0 \text{ and } m = 2.2 \tag{22}$$

Heat Transfer: The overall heat transfer to the cylinder gases is given by

$$\dot{Q} = h_c A(\theta) (T_{wall} - T_{avg}) \tag{23}$$

Note that the overall heat transfer is based on the cylinder average gas temperature (T_{avg}), and the total surface area (A). During the combustion process, the total heat transfer is allocated to the various zones (but the total is

still given by eq. 23). This allocation may be completed in a number of ways. For this work, the heat transfer is assumed to be proportional to the surface area of each zone. The appropriate surface area is assumed to be proportional to the volume raised to the 2/3 power. In addition, the heat transfer is proportional to the temperature difference. For example, since the unburned zone temperature is lower, the proportion of the heat transfer allocated to the unburned zone should be lower as well. This results in the following for the individual allocated heat transfer values,

$$\dot{Q}_u = \left(\frac{V_u}{V_{total}} \right)^{2/3} \left(\frac{T_{wall} - T_u}{T_{wall} - T_{avg}} \right) \dot{Q}_{total} \quad (24)$$

$$\dot{Q}_b = \dot{Q}_u - \dot{Q}_{total} \quad (25)$$

Since the burned zone is divided into an adiabatic core and a boundary layer, the burned zone heat transfer is assigned in total to the boundary layer.

A number of correlations for the instantaneous convective heat transfer coefficient (h_c) have been proposed and used throughout the years. The current work has used the correlation proposed by Woschni (1968).

Mass Flow Rates: The mass flow rates are based on assumptions and approximations which include that the flow is quasi-steady, one-dimensional, adiabatic and reversible. These assumptions and approximations are corrected by use of an empirical discharge coefficient. For purposes of this study, the discharge coefficient has been assumed constant with a value of 0.7, which is a typical average value (Heywood, 1988).

Finally, the open flow area is needed which depends on the valve diameter and instantaneous valve lift. Since the valve lift profiles are not necessarily known, this work has used a standard assumption for the valve lift based solely on the maximum lift and the valve open duration, and using a sinusoidal shape as recommended by Sherman and Blumberg (1977).

Mass Conservation: In addition to the energy equation described above, mass conservation must be satisfied throughout the computation. The instantaneous change in

the cylinder mass is equal to the net result of the mass flow rates:

$$\frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out} \quad (26)$$

Numerical Solution: The instantaneous cylinder conditions (temperatures, pressure, volumes, masses, and thermodynamic properties) as a function of crank angle are obtained by the simultaneous numerical integration of the various differential equations. Since a number of the differential equations are themselves dependent on the other variables, an iterative approach was chosen. That is, the set of differential equations were evaluated, and then these values were used to determine the “final” values of the derivatives. For the two zone portion (eq. 10), two iterations were sufficient for convergence. For the three zone portion (eq. 18), four iterations were necessary.

A number of numerical methods are available to solve a set of differential equations like the ones outlined above. Both the Runge-Kutta technique and a simple Euler technique were evaluated. The two methods provided surprisingly similar results. Since the application of the Euler technique was more straightforward, it was selected for this work. A description of the sensitivity to the time step interval for the calculations is presented in the subsequent results section.

The current formulation of this cycle simulation was developed using FORTRAN. Specifically, the “Digital Visual Fortran,” from Digital Equipment Corporation, Inc., was used. This software currently is issued by Compaq, Inc.

To complete the required input information, the boundary conditions for the inlet (temperature and pressure) and for the exhaust (pressure) are specified. To begin a particular engine cycle calculation, several parameters are not known. The initial amount of exhaust gases (residual), and the initial cylinder gas temperature and pressure must be assumed. The complete calculation is repeated until the final values agree with the initial values. Depending on the specified tolerance, this procedure usually finds convergence within about three (3) complete cycles.

Table 1. Engine Specifications

Item	Heywood <i>et al.</i> (1979)	Current
Number of cylinders	8	8
Bore (mm)	101.6	101.6
Stroke (mm)	88.4	88.4
Crank Rad/Con Rod	0.305	0.305
Compression Ratio	8.1:1	8.1:1
Inlet Valves:		
Diameter (mm)	50.8	50.8
Max Lift (mm)	9.75	10.0
Opens (°CA aTDC)	346	357
Closes (°CA aTDC)	-116	-136
Exhaust Valves:		
Diameter (mm)	39.6	39.6
Max Lift (mm)	10.3	10.0
Opens (°CA aTDC)	116	116
Closes (°CA aTDC)	386	371
Valve Overlap (degrees)	40°	14°
Heat Transfer Multiplier	n/a	1.33

Checks: A number of internal consistency checks may be used. For example, the overall mass balance and energy equation may be used as a check:

$$m_b u_b = m_a u_a + m_{bl} u_{bl} \quad (27)$$

Also, a number of individual mass balances and the use of the ideal gas relation may be used as additional checks.

ENGINE AND OPERATING SPECIFICATIONS

The selected engine was a 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. This engine was the one used by Heywood *et al.* (1979) in a set of related studies. The results presented below are for a part load operating condition at 1400 rpm with an equivalence ratio of 1.0.

Table 2. Engine Input and Other Parameters

Item	Value Used	How Obtained
Displaced Volume (dm ³)	5.733	Computed
AF	15.13	For isooctane, ref. A*
Frictional mep (kPa)	72.4	From ref. B**
Inlet Pressure (kPa)	52	Inferred from Fig. 10 in ref. B
Exhaust Pressure (kPa)	105	Estimated
Engine Speed (rpm)	1400	From ref. B
Combustion duration (°CA)	60	From ref. B
Inlet Temperature (K)	319	From ref. B
Cylinder Wall Temp (K)	450	Estimated
Fuel LHV (kJ/kg)	44,400	From ref. B

*Ref. A: Heywood (1988)

**Ref. B: Heywood *et al.* (1979)

Table 1 lists the engine specifications as provided by Heywood *et al.* (1979), and as used in the present work (current). Using the listed valve timings resulted in excessive back flow and unrealistic flow characteristics during the valve overlap period. To avoid excess back-flow, the amount of valve overlap was reduced. As shown, the intake valve open and close crank angles, and the exhaust valve close crank angle were modified. The overall valve overlap was decreased from the apparent 40° to 14°. This provided much more realistic flow rates which agreed with those published (see following). The reasons for the need for this valve timing modification included the fact that the original modeling work (Heywood, *et al.*, 1979) used actual cam profiles whereas the current work used a “sinusoidal” cam profile (since the actual cam profiles were not available). Further, the actual valve timings used in the original modeling work (Heywood, *et al.*, 1979) may have differed from those which were listed as the engine specifications.

Finally, the table lists an empirical heat transfer multiplier which was set to 1.33 to provide good agreement with the published results. The need for this “multiplier” may be due to a difference in the implementation of the original heat transfer algorithm, or a similar constant used by the original investigators, but not reported. Using this

“multiplier,” the final results for the heat transfer are in good agreement with the published results.

Table 2 lists other parameters (and their source) which were needed in this work. Although most of the significant engine parameters were duplicated in an exact fashion by the current study, a few parameters were estimated, inferred or interpreted from figures, or modified. The parameters affected included items such as the valve timings, the valve lift profiles, the exhaust and inlet pressures, the unused fuel, and the cylinder wall temperature. In gener-

al, modest changes in these parameters will not significantly change the results of the current study.

RESULTS AND DISCUSSION

Results from this project are described in the following five sections:

1. Studies of the use of exhaust gas recirculation
2. Studies of the use of hydrogen
3. Studies of the use of the alcohol fuels
4. Studies of compression ratio and expansion ratio
5. Studies of the use of turbocharging

Section 1: Use of Exhaust Gas Recirculation

The major motivation for using EGR in reciprocating, internal-combustion engines is to reduce nitric oxide (NO) emissions. An additional benefit of the use of EGR are improvements in engine thermal efficiency due to improved thermodynamic characteristics. The disadvantages include a decrease of engine power density at wide open throttle (WOT).

This study is an examination of the effects of exhaust gas recirculation (EGR) on engine performance, available energy, and nitric oxide emissions for a spark ignition engine. The objective of this work is to quantify these expectations for a specific part-load operating condition.

The percentage of EGR for this work is defined as:

$$EGR = \frac{m_{EGR}}{m_{inlet}} \times 100\%$$

where m_{EGR} is the mass per cycle of the exhaust gas recirculated, and m_{inlet} is the total mass (EGR + air + fuel vapor) per cycle which enters the engine. Any residual gases retained in the cylinder are additional sources of burned gas, are automatically included in the computations, and vary with each operating condition. The following computations do not consider combustion stability, cycle-to-cycle variations, or other combustion quality issues as the EGR level increases. For conventional SI engines, the maximum EGR level is typically limited from 15% to 30%. For higher levels of EGR, the combustion quality begins to deteriorate and combustion stability becomes an issue. Higher levels of EGR are often possible, however, by the use of fast burn combustion designs. A relatively wide range of EGR levels is considered in these computations to better illustrate the trends with respect to increases of EGR. These higher levels of EGR may or may not be practical in actual applications. In addition, the following computations do not consider the possibility of spark knock or preignition.

Two EGR configurations were considered: (1) a cooled configuration and (2) an adiabatic configuration. These two configurations provide inlet mixture temperatures that bracket the range of possible inlet mixture temperatures when using EGR.

Figure 1 shows the inlet mixture temperature as functions of the percentage of EGR for the base case for the two EGR configurations. The inlet mixture temperature is constant (with a value of 319.4 K) as the percentage of EGR increases for the cooled configuration. For the adiabatic EGR configuration, the inlet mixture temperature increases as the percentage of EGR increases. As the percentage of EGR increases, the exhaust gas temperature decreases, and therefore, the rate of increase of the inlet mixture temperature decreases for higher EGR levels. For these conditions, for EGR levels greater than about 30%, the inlet mixture temperature increases relatively little for further increases in EGR levels. For 40% EGR, the inlet mixture temperature is about 460 K for these conditions.

Figure 1. Inlet mixture temperature as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

Table 1 is a list of some of the parameters for the base case conditions. In general, the start of combustion (θ_c) needed to be advanced as EGR levels increased to maintain "MBT" performance. Also, as EGR levels increased, the inlet manifold pressure (p_{in}) needed to increase to maintain the constant bmep.

First, to demonstrate the effectiveness of EGR for reducing nitric oxide emissions, figure 2 shows the nitric oxide concentrations as functions of the percentage of

EGR for the base case for the two EGR configurations. The nitric oxide concentration decreases rapidly with increasing EGR. The cooled EGR configuration results in lower nitric oxide emissions relative to the adiabatic EGR configuration since the gas temperatures (described below) are lower. Even for the adiabatic EGR configuration, however, over 90% reduction in nitric oxide is obtained with about 25% EGR.

Table 1. Base Case Parameters
(1400 rpm, bmep = 325 kPa, $\phi = 1.0$)

Item → Case ↓	EGR (%)	θ_o (relative to TDC)	p_{in} (kPa)	p_{exh} (kPa)	$T_{in,mix}$ (K)
No EGR	0	-20.5	50.1	102.6	319.4
Cooled	10	-21.0	53.6	102.8	319.4
Cooled	20	-21.0	58.0	103.0	319.4
Cooled	30	-21.5	63.5	103.4	319.4
Cooled	40	-22.0	70.7	103.9	319.4
Adiabatic	10	-24.0	62.0	103.3	390.4
Adiabatic	20	-25.0	72.9	104.0	434.7
Adiabatic	30	-26.0	83.3	104.9	456.4
Adiabatic	40	-26.5	93.5	105.8	459.6

Figure 3 shows the indicated and brake thermal efficiencies as functions of the percentage of EGR for the base case for the two EGR configurations. Both the indicated and brake efficiencies increase with increasing percentage of EGR, and the results are similar for the two EGR configurations. The brake thermal efficiency is slightly higher for the cooled EGR case. The brake thermal efficiency increases from about 25.7% to about 29% as EGR increases from 0 to 40%. These increases of the thermal efficiencies for the use of EGR are the result of lower gas temperatures, lower heat transfer, favorable thermodynamic properties, reduced dissociation near top dead center, and lower pumping losses (a consequence of the constant load condition). These items are quantified in the following discussion. The reasons for the similar results for the two EGR configurations are explained

below in terms of the various energy and availability terms.

Figure 2. Specific nitric oxide concentration in the exhaust as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

Figure 4 shows the maximum cylinder gas temperatures, average gas temperatures during the combustion process, and average exhaust gas temperatures as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations. The maximum cylinder gas temperature was a single (spatial average) temperature that typically occurred at about 22–29°aTDC (depending on conditions). The two average gas temperatures are based on an energy-weighted average. In general, all three temperatures decrease as the percentage of EGR increases, and the three temperatures are higher for the adiabatic configuration relative to the cooled configuration, as expected.

Figure 3. Indicated and brake thermal efficiency as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

Figure 5 shows three availability terms as functions of the percentage of EGR for the base case for the two EGR configurations. The majority of the availability of the fuel is distributed between these three terms and the indicated work. The indicated work is proportional to the indicated thermal efficiency. These results can best be explained by knowing the changes in the various gas temperatures (figure 4). The three availability terms will be discussed in this order: (1) the availability destroyed by the combustion process, (2) the availability moved to the cylinder walls via heat transfer, and (3) the net availability leaving the cylinder with the exhaust gases.

Figure 4. Maximum cylinder gas temperatures, average gas temperatures during the combustion process, and average exhaust gas temperatures as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

Figure 5. Three availability terms as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

For EGR levels greater than about 10%, the availability destroyed by the combustion process increases with increases in the percentage of EGR. This is a direct consequence of the decrease in the combustion gas temperatures. Further, the availability destroyed by the combustion process is higher for the cooled EGR configuration since this configuration results in lower combustion gas temperatures than for the adiabatic EGR configuration. For the adiabatic EGR configuration for EGR levels less than about 10%, the availability destroyed by the combustion process slightly decreases with increases in the percentage of EGR. For this configuration (adiabatic) and this range of EGR levels, the average combustion gas temperature is essentially constant. The slight decrease of the availability destroyed by the combustion process is due to the change in the thermodynamics.

For EGR levels greater than about 12%, the availability moved to the cylinder walls via the heat transfer decreases as the percentage of EGR increases. This is due to the lower gas temperatures as the percentage of EGR increases which decreases the temperature difference and hence decreases the heat transfer rates. The adiabatic EGR configuration results in more availability moved to the cylinder walls than the cooled EGR configuration since the adiabatic EGR configuration results in the higher gas temperatures. For the adiabatic EGR configuration for EGR levels less than about 12%, the availability moved to the cylinder increases as the percentage of EGR increases. Again, for this configuration (adiabatic) and this range of EGR levels, the average combustion gas temperature is essentially constant. The increase of the availability moved to the cylinder walls is due to the increase in the heat transfer coefficient² as EGR levels increase due to the decrease of the gas temperatures and the associated change in the thermodynamic properties. This increase of the heat transfer coefficient as EGR levels increase continues for higher levels of EGR (greater than 12%), but the relative importance of the temperature decrease in this range (12% to 40%) dominates the slight increase of the heat transfer coefficient.

Returning to figure 5, the “net” availability leaving the cylinder with the exhaust gases refers to the difference between the availability leaving (exhaust) and entering (intake charge). The net availability leaving the cylinder with the exhaust gases decreases as the percentage of EGR increases. The difference between the average exhaust gas temperature and the inlet mixture temperature as the percentage of EGR increases for the two EGR configurations decreases as the percentage of EGR increases. Further, the cooled EGR case results in a higher temperature difference than the adiabatic case. This is because for the adiabatic EGR case, the inlet mixture temperature increases more (relative to the cooled EGR case) than the ex-

haust temperature increases (relative to the cooled EGR case). The net availability leaving the cylinder is higher for the cooled EGR case since this case has a higher net temperature difference.

Figures 6 and 7 are another way to illustrate these results. These figures show the percentage of the fuel availability that is distributed between indicated work (100% availability), availability moved to the cylinder walls via heat transfer, net availability in the exhaust, availability destroyed by combustion, availability destroyed by mixing and unused availability (unburned fuel). Figures 6 and 7 show these results for the adiabatic and cooled configurations, respectively, for 0% and 40% EGR. (The 0% EGR case is the same for both configurations). The major differences between the two configurations are that the adiabatic EGR case, relative to the cooled EGR case, has lower combustion destruction and lower availability in the exhaust, but higher availability moved via heat transfer. As mentioned above, the overall results, such as indicated thermal efficiency, is almost the same for the two EGR configurations.

Finally, these results may be used to help explain the results of figure 4 which showed the thermal efficiencies were similar for both the cooled and adiabatic EGR configurations. For the adiabatic EGR case (relative to the cooled EGR case), the combustion destroyed availability and the net availability that leaves the cylinder with the exhaust gases are less, but the availability moved to the cylinder walls via heat transfer is higher. For the cooled EGR case (relative to the adiabatic EGR case), the availability moved to the cylinder walls via heat transfer is much less, but this is balanced by the higher amounts of availability in the exhaust and destroyed by the combustion process. The net effect, at least for these conditions, is that the thermal efficiencies are about the same for both EGR configurations.

These results for the use of EGR were compared to results for oxygen enriched inlet air. Since the use of EGR is effectively reducing the oxygen concentration of the inlet mixture, these results should be related to the results for the use of inlet air with oxygen enrichment. The use of inlet air with oxygen enrichment is a technique that has been previously studied using the cycle simulation for similar conditions [7]. Figure 8 shows the percentage of the fuel availability destroyed by the combustion process as functions of the oxygen volume percent. For the cases with oxygen percentages greater than 21%, the inlet air was enriched with additional oxygen (and no EGR was used). The combustion destruction of availability is reduced for increasing levels of oxygen due to the higher combustion temperatures and the reduced mixing losses associated with the lower nitrogen content for higher oxygen enrichment. These results have been documented elsewhere [7].

² The heat transfer coefficient is inversely dependent on gas temperature (to a fractional power) – so, for decreasing gas temperatures (as EGR levels increase), the heat transfer coefficient increases slightly.

Figure 6. Percentage of the fuel availability for various items for the base case conditions for 0% and 40% EGR for the adiabatic EGR case.

Figure 7. Percentage of the fuel availability for various items for the base case conditions for 0% and 40% EGR for the cooled EGR case.

For the cases with oxygen percentages less than 21%, the use of EGR causes a reduction in the oxygen concentration of the inlet charge. The top scale in figure 8 shows the percentage EGR which corresponds to the bottom scale of oxygen concentration. Both the adiabatic and cooled EGR configurations have been examined. The cooled EGR configuration results in increases in the combustion destruction as EGR increases (as shown above). The relationship is continuous with the oxygen enrichment results (oxygen concentration greater than 21%). Finally, for the adiabatic configuration, the results for the combustion destroyed generally increase as EGR

increases, but these results are not continuous with the results for the oxygen enrichment results. The curvature of these results for the adiabatic configuration has been explained above.

Figure 8. Combustion destroyed availability as functions of oxygen concentration in the inlet mixture for the base case conditions using either EGR or oxygen enrichment.

Conclusions: This section has examined the use of exhaust gas recirculation (EGR) for a spark-ignition engine at a part load operating condition. A cooled and an adiabatic EGR configuration were studied. The cycle simulation results demonstrated an increase in thermal efficiency for increasing levels of EGR. In addition, the results from a second law analysis indicated that the destroyed availability due to combustion increased with increasing levels of EGR. These results were shown to be largely a result of reduced heat losses as the EGR levels increased. For an operating condition which included an EGR level of 20%, an equivalence ratio of 1.0, MBT spark timing, 1400 rpm, and a brake mean effective pressure of 325 kPa, the destroyed availability due to combustion was 20.7% and 22.5% of the fuel's original availability for the adiabatic and cooled configurations, respectively.

Section 2: The Use of Hydrogen

The use of hydrogen as a fuel for internal combustion engines began in the 1800s during the development of the first IC engines [1]. As an example, an engine developed by Cecil in 1820 has been credited with using hydrogen [1]. The use of hydrogen as an IC engine fuel has been studied throughout the years as a response to the need for a substitute for petroleum fuels, and as an environmentally cleaner fuel. Periods of more intense work on this topic include the time around the two world wars (~1920s and ~1940s), and around the oil shortages of the 1970s and 1980s. The current interest in using hydrogen as a fuel for internal combustion engines has been motivated by a desire to reduce the nation's dependence on petroleum fuels, to use a fuel that does not produce carbon dioxide (a "green-house" gas), and to minimize regulated emissions.

The literature on the use of hydrogen in IC engines is vast, and the following is not an attempt to be comprehensive, but rather, to provide examples of some of the work that has been completed on this topic.

deBoer *et al.* [1] published a description of the potential benefits of operating IC engines with hydrogen. They suggested that the use of unthrottled, lean mixtures would result in high thermal efficiencies. They proposed methods to avoid knock, preignition, and back-fire. Shelef and Kukkonen [2] provide an assessment of the potential for hydrogen to serve as a fuel for automotive engines.

More recently, Karim [3] and Sierens *et al.* [4] have provided overviews of the state of the technology. These references discuss the various aspects of hydrogen as an engine fuel. Some of the more unique features of hydrogen as an engine fuel are high flame speeds, wide flammability limits, and high octane number. These features have a dramatic impact on engine operation. For example, the robust combustion of hydrogen means that higher dilution (e.g., exhaust gas recirculation) can be tolerated, and cycle-to-cycle variability will be minimized [5].

Although hydrogen has some attractive features as an engine fuel, there are a number of concerns with the use of hydrogen. Because of the wide flammability limits of hydrogen

, back fire and preignition are potential problems [1–8]. If not controlled, the rapid burning can result in excessive cylinder pressures and temperatures, and high heat losses.

The objectives of the current work are to compare the performance and second law parameters of a conventional spark-ignition engine operated on isooctane or hydrogen. The comparisons will include three forms of hydrogen operation which take advantage of the above features of hydrogen as an engine fuel.

Engine Optimization Strategies: As mentioned above, hydrogen has certain features which can be used for unique load control for a naturally aspirated, spark-ignition engine [4]. For example, a spark-ignition engine could be designed to operate as much as possible with wide open throttle, and then load would be controlled with changes in the equivalence ratio. For the lowest loads, some throttling may be necessary to maintain stable combustion.

In addition, an engine could be designed with a high compression ratio since hydrogen has a high effective octane rating [8]. This will increase the thermal efficiency relative to using conventional hydrocarbon fuels. In yet another type of optimization, a hydrogen engine could be designed to result in the lowest emissions. For each application, therefore, a wide range of combinations are possible for the selection of operating conditions (including items such as equivalence ratio, inlet pressure, exhaust gas recirculation, and spark timing), and design parameters (such as compression ratio and valve timings). The final selection will be dictated by the relative importance of the goals of performance, fuel efficiency, and low emissions. No unique set of these conditions and parameters have been identified as universal.

Results: First, limitations of the current study are discussed. Next, a description of the operating conditions for each of the cases studied is described. Then the results from this study are presented in the following five sections: (1) time-resolved results, (2) base case results, (3) engine performance results, (4) second law results, and (5) nitric oxide emissions results.

Limitations of Study: This initial study is aimed at providing consistent comparisons of engine operation using either isooctane or hydrogen. For this reason, the selection of operating conditions may not be optimal. For ex-

ample, hydrogen may be used in an “unthrottled” operating mode, and equivalence ratio would be used for load control. Also, a hydrogen engine would perhaps be designed with a higher compression ratio than an isooctane engine. Some operating strategies may use EGR to reduce nitric oxide emissions. For consistent comparisons, however, this initial study has elected to consider the same compression ratio, and generally the same operating conditions. Future studies will be directed to complete these same type of comparisons, but based on engine conditions and parameters that are more optimal for the hydrogen case.

One area of concern is the burn duration assigned for hydrogen combustion. Caton (2006) contains a description of results for hydrogen which examine in some detail the importance of burn duration and equivalence ratio on engine performance.

Description of Cases: The use of hydrogen alters several aspects of the engine thermodynamics. One difference is that for part load operation, the hydrogen engine requires a higher inlet pressure for equal power (all else the same). In addition, the use of hydrogen is expected to result in higher flame speeds and shorter combustion durations [1–8]. These two aspects are reflected in the following results.

To begin, two cases for hydrogen will be considered for comparison with an isooctane case. In all cases, the start of combustion will be adjusted (“MBT” timing) to obtain the highest bmep for that condition. Both the isooctane case and the first hydrogen case will be based on a combustion duration of 60°.

The second hydrogen case is based on a shorter combustion duration. Hydrogen is expected to have a much faster burn process. The burn duration for hydrogen for typical engine conditions could be about one-half or less relative to the value for gasoline fuels [1–8]. To examine the effect of the shorter burn duration, results were obtained for the same conditions, but with a burn duration of 30°CA. For this shorter burn duration, the start of combustion was adjusted significantly to provide “MBT” timing.

These results are for premixed mixtures of fuel vapor and air. Table 2 lists some of the basic engine inputs and some of the basic engine results for the part-load base case operating condition. Due to the higher

stoichiometric air-fuel ratio for hydrogen relative to isooctane (34.3 vs. 15.1), to produce an equal engine output (say, bmep), the hydrogen-fueled engine requires a higher inlet manifold pressure (all else equal). Table 2 lists an inlet pressure of 59.9 and 59.4 kPa for the two hydrogen cases relative to 50.0 kPa for the isooctane case.

**Table 2. Base Case Engine Inputs and Results
(Base Case: 1400 rpm, “MBT” timing, $\phi = 1.0$)**

Item	C ₈ H ₁₈ ($\theta_b=60^\circ$)	H ₂ ($\theta_b=60^\circ$)	H ₂ ($\theta_b=30^\circ$)
Displaced Volume (dm ³)	5.733	5.733	5.733
Engine Speed (rpm)	1400	1400	1400
bmep (kPa)	325	325	325
Combustion duration (°CA)	60	60	30
Inlet Temperature (K)	319	319	319
Cylinder Wall Temp (K)	450	450	450
Inlet Pressure (kPa)	50.0	59.9	59.4
Start of Combustion (°bTDC)	20.5	20.5	5.5
AF _{stoich}	15.13	34.32	34.32
Fuel LHV (kJ/kg)	44,400	120,000	120,000
Mechanical Friction mep (kPa)	68.5	70.0	69.9
Exhaust Pressure (kPa)	102.6	103.2	103.1
Residual fraction	0.1074	0.1066	0.1083
Nitric oxide emissions (ppm)	2973	4612	4892

The “MBT” start of combustion is the same (at 20.5°bTDC) for the isooctane case and the first hydrogen case, but (due to the shorter burn duration) the second hydrogen case has a start of combustion much retarded (at 5.5°bTDC).

Figure 2. Cylinder pressure as functions of crank angle for the three cases.

Time-Resolved Results: Figures 2 and 3 show the cylinder pressures and the one-zone, average cylinder gas temperatures, respectively, as functions of crank angle for the three cases. The lowest pressures and temperatures are generally for the isooctane case, and the highest pressures and temperatures are for the “fast-burn” hydrogen case with the normal hydrogen case in between the other two. For the constant load condition of this comparison, the cases for hydrogen fuel have higher pressures and temperatures due largely to the net higher amount of energy release (per mass of air) during the combustion process. Compared to isooctane, hydrogen has about 20% more energy release per mass of air for stoichiometric combustion. This results in higher combustion temperatures, which results in higher heat transfer and lower thermal efficiency. The net result is the need for higher cylinder pressures to provide equal power. This means that the indicated thermal efficiency is higher for the hydrogen cases compared to the isooctane case.

Figures 4–6 show the flow rates as functions of crank angle for the three cases. The general nature of the flow rates is similar for the three cases. For the same load (bmep), the flow rates for the isooctane case are slightly

Figure 3. One-zone cylinder gas temperatures as functions of crank angle for the three cases.

higher than for the hydrogen cases. This is the net result of the different heating values and stoichiometric ratios. When the intake valve opens, the flow is back into the manifold since the cylinder pressure is greater than the manifold pressure. After about 374 CA°aTDC, the flow is into the cylinder from the manifold. The first gases into the cylinder are residual gases which were just placed in the manifold during the back-flow. After those gases have entered the cylinder, then the fresh charge starts to enter the cylinder (usually about 400°aTDC for these cases).

Figures 7–9 show the one-zone, average cylinder gas temperature as functions of the cylinder gas specific entropy for the three cases. The numbers on the curves denote the crank angle. The entropy is nearly constant or slightly decreases (due to heat loss) during the compression process, but the temperature increases. Once combustion starts, the entropy and temperature increase. Shortly before the end of combustion, the temperature starts to decrease. The temperature and entropy decrease during the expansion process. Once blow-down ends, the entropy decreases much more quickly, and the temperature decreases much more slowly. Once the

fresh charge begins to enter the cylinder, the temperature and entropy decrease until they reach their starting values.

The two hydrogen cases (figures 8 and 9) are a little different compared to the isooctane case. After the exhaust valve closes, the entropy increases slightly during the period when the residual gases are returning to the cylinder. These gases have a greater entropy than the cooled cylinder gases so the entropy increases. Once the fresh charge begins to enter the cylinder, the entropy (and temperature) continue to decrease until they reach their initial values at intake valve closing.

Figure 4. Flow rates, and cylinder pressures and temperatures as functions of crank angle for the isooctane case.

Figure 5. Flow rates and cylinder pressures and temperatures as functions of crank angle for base hydrogen case.

Figure 6. Flow rates and cylinder pressures and temperatures as functions of crank angle for the fast-burn hydrogen case.

Figure 7. One-zone, average cylinder gas temperature as functions of cylinder gas specific entropy for the isooctane case.

Figure 9. One-zone, average cylinder gas temperature as functions of cylinder gas specific entropy for the fast-burn hydrogen case.

Figure 8. One-zone, average cylinder gas temperature as functions of cylinder gas specific entropy for the base hydrogen case.

Base Case Results: Again, table 2 lists some of the base case engine results for the part-load operating condition. Table 2 also lists the nitric oxide emissions for the three cases. Both hydrogen cases result in much higher (55% and 65% higher, respectively) nitric oxide emissions compared to the isooctane case. This is a direct result of higher gas temperatures which are examined below. Additional nitric oxide results are presented in a following section.

Table 3 lists the distribution of the fuel energy among the major energy items for the three cases. The brake power percentage is the brake thermal efficiency. The brake efficiency is slightly higher for the isooctane case primarily because of the lower gas temperatures and lower heat loss. Roughly, the brake thermal efficiency is about 25%, the heat loss is about 28%, and the energy in the exhaust is about 41% for this operating condition for all three cases.

Table 4 shows the distribution of the fuel availability among four major items for the three cases. (The distribution of the availability as a function of load is described in a following section). The two hydrogen cases

are similar, but they are different than the isooctane case. The percentage of the fuel availability that is used as indicated power (similar to the indicated thermal efficiency) is about 30.3% for the isooctane case and about 31.7% and 32.2% for the two hydrogen cases. The percentage availability that leaves due to heat transfer is about 22.1% for the isooctane case, and about 25.0% for the two hydrogen cases. The availability retained in the exhaust gases is about 24.6% for the isooctane case, and about 30% for the two hydrogen cases. Finally, the percentage availability destroyed by the combustion process is about 21% for the isooctane case, and about 11% for the hydrogen cases.

Table 3. Base Case Energy Results
(Base Case: 1400 rpm, "MBT" timing, $\phi = 1.0$)

Item	C_8H_{18} ($\theta_b=60^\circ$)	H_2 ($\theta_b=60^\circ$)	H_2 ($\theta_b=30^\circ$)
	(Percentage of Fuel Energy)		
Brake Power	25.67	24.71	24.98
Mechanical Friction	5.41	5.32	5.37
Heat Loss	27.46	27.89	28.09
Exhaust	40.79	41.40	40.89
Unburned	0.69	0.69	0.67

Table 4. Base Case Availability Results
(Base Case: 1400 rpm, "MBT" timing, $\phi = 1.0$)

Item	C_8H_{18} ($\theta_b=60^\circ$)	H_2 ($\theta_b=60^\circ$)	H_2 ($\theta_b=30^\circ$)
	(Percentage of Fuel Availability)		
Indicated Power	30.28	31.74	32.21
Heat Loss	22.13	24.64	25.03
Comb Avail Destruct	21.00	11.04	10.65
Exhaust	24.56	30.06	29.84
Intake Mixing Destru	1.37	1.84	1.60
Unburned	0.67	0.68	0.68

In general, the availability results in table 4 are largely consequences of the higher cylinder gas temperatures associated with the hydrogen cases. These higher temperatures result in the lower destruction of availability due to combustion, but result in higher heat losses and more availability retained by the exhaust gases. Additional second law results are presented in a following sub-section.

Engine Performance Results: The next set of results show engine performance as functions of the engine load as represented by the bmep. One new hydrogen case is introduced, and the details of this case are described in a subsequent part of this sub-section.

Figure 10 shows the brake thermal efficiency as functions of engine load (bmep) for the three previous cases ($\phi = 1.0$) and for the new hydrogen case ($\phi \leq 1.0$). For the three previous cases, the brake thermal efficiency increases as engine load increases for all cases due largely to the decreasing throttle losses (pumping work) and decreasing relative heat losses. The thermal efficiency is highest for the isooctane case due primarily to the lower heat losses. The thermal efficiency for the fast-burn hydrogen case is slightly higher than for the normal burn hydrogen case.

In addition, the use of isooctane results in a higher maximum load (maximum bmep of about 886 kPa) relative to the use of hydrogen (maximum bmep of about 684 kPa). This result is due to the lower volume of fuel vapor for the isooctane stoichiometric operation compared to stoichiometric hydrogen operation.

Figure 10. Brake thermal efficiency as functions of brake mean effective pressure for the base case using isooctane and three cases using hydrogen.

Figure 10 also includes results for the new additional hydrogen case which is based on a burn duration of 30° (fast burn). For this case, the advantages of the lean flammability characteristics of hydrogen are used for all but the WOT condition. For these computations, the assumption was that the lean limit for hydrogen mixtures is an equivalence ratio of 0.4. This may be aggressive, but the intention is to illustrate the concept.

Figure 11 shows the equivalence ratio (ϕ) and inlet pressure (p_{in}) as functions of load (bmep) for this case. For loads less than a bmep of 353 kPa, a lean mixture with an equivalence ratio of 0.4 was used. As load increased from idle, the throttle was opened. At a bmep of 353 kPa, the throttle was wide open (WOT), and the equivalence ratio was 0.4. For higher loads (bmep > 353 kPa), the equivalence ratio was increased from 0.4 to 1.0 (maximum bmep condition). The brake thermal efficiency was highest for this case as compared to the other three cases. The use of hydrogen with variable equivalence ratio results in the highest efficiencies with a maximum brake thermal efficiency of about 32.0%. The strat-

egy of this case provides gains in brake thermal efficiency due to the favorable thermodynamics and low temperatures of lean combustion.

Figure 11. Equivalence ratio and inlet manifold pressure as functions of engine load (bmep) for the fast-burn hydrogen case with variable equivalence ratio.

Figure 12 shows the brake specific fuel consumption (*bsfc*) as functions of engine load (*bmep*) for the three cases. As engine load increases, the *bsfc* decreases which reflects the decrease of pumping losses (throttle opens). In general, the *bsfc* is the inverse of the thermal efficiency. In this case, however, since the molecular mass of hydrogen is smaller than for the isooctane, the *bsfc* values are lower for hydrogen than for isooctane.

Another way to examine these results is to consider the brake specific fuel energy consumption. Figure 13 shows the brake specific fuel energy consumption as functions of engine load (bmep) for the three cases. In this format, the three curves are nearly the same which is similar to the results in figure 10 for the thermal efficiency.

Second Law Results: Figures 14 to 17 show the distribution of the fuel availability among the engine quantities as functions of the engine load (bmep) for the four cases. In general, the brake and indicated work increase with increasing load largely due to less throttle losses. The fraction of the availability that is moved out of the system

Figure 12. Brake specific fuel consumption as functions of brake mean effective pressure (bmep) for the base case using iso-octane and the two cases using hydrogen.

due to heat transfer decreases as load increases. Although the absolute heat transfer increases with load (due to the higher gas temperatures), the fueling increases at a faster rate. The net effect is that the (relative) heat transfer as a fraction of the fueling decreases with increases in load. The fraction of the availability that is in the exhaust slightly increases with load. Since the relative heat transfer and pumping work are decreasing with load, additional energy and availability is retained in the exhaust gases. Finally, the fraction of the availability destroyed by combustion remains nearly constant as load increases for these conditions. The trends of the results are similar for both fuels as functions of load.

Figure 16 shows the distribution of availability as a function of engine load for the hydrogen case with the shorter burn duration (30°CA) with all other conditions as before. In general, the results are similar for the two burn durations. The case with shorter burn duration does result in a slight increase in the brake thermal efficiency.

Figure 17 shows the distribution of availability as a function of engine load for the strategy with variable equivalence ratios for engine loads (bmep) greater than 353 kPa, and an equivalence ratio of 0.4 for engine loads (bmep) less than 353 kPa. These results are for the shorter burn duration of 30°CA and with all other conditions as before. The highest brake efficiency is about 32.0% for the engine load of 353 kPa where the throttle is still wide open and the equivalence ratio is 0.4. For lower loads, the throttle is closing, and for higher loads the equivalence ratio is increasing. For the highest efficiency condition (bmep = 353 kPa), the availability in the exhaust gases and associated with the heat transfer are minimum. On the other hand, the availability destroyed by combustion is minimum (with a value of about 11.0%) for the full load condition.

Figure 13. Brake specific energy consumption as functions of brake mean effective pressure (bmep) for the base case using iso-octane and the two cases using hydrogen.

Figure 14. Availability distribution as functions of engine load (bmep) for the isooctane base case.

Figure 16. Availability distribution as functions of engine load (bmep) for the fast-burn hydrogen base case.

Figure 15. Availability distribution as functions of engine load (bmep) for the hydrogen base case.

Figure 17. Availability distribution as functions of engine load (bmep) for the fast-burn hydrogen case with variable equivalence ratio.

Figure 18. The distribution of energy and availability for engine operation with **isooctane** with a burn duration of 60° for a bmep of 325 kPa, an equivalence ratio of 1.0, and 1400 rpm.

Figure 19. The distribution of energy and availability for engine operation with **hydrogen** with a burn duration of 60° for a bmep of 325 kPa, an equivalence ratio of 1.0, and 1400 rpm.

Figures 18 and 19, for isooctane and hydrogen, respectively, show the distribution of availability (right) and energy (left) for the base conditions. For isooctane (figure 18), the total indicated work on an energy basis was 31.1% and was 30.3% on an availability basis. The heat transfer was 27.5% of the original energy, but only 22.1% of the availability. In the exhaust, the net energy was 40.7%, and the net availability was 24.4%. Combustion destroyed 21.1% of the availability. In contrast, figure 19 shows the results for hydrogen. On an energy ba-

sis, the numbers are similar. On an availability basis, however, more availability is retained in the exhaust (30.4%) and less is destroyed by combustion (11.2%). For the hydrogen cases, preserving availability by reducing the destruction during combustion results in an increase of the availability in the exhaust and not additional work.

Figure 20 shows the destroyed availability due to combustion as functions of the engine load for the isooctane and the two hydrogen cases. The destroyed availability increases slightly with increasing load for the hydrogen cases, and decreases slightly for the isooctane case. The two hydrogen cases have between about 10–11.5% destruction, and the isooctane case has between about 20.8–21.3% destruction for the conditions examined.

Figure 20. The destroyed availability due to combustion as functions of engine load (bmep) for engine operation with hydrogen with a burn duration of 60°, with hydrogen with a burn duration of 30° (fast burn), and with isooctane for an equivalence ratio of 1.0, and 1400 rpm.

Nitric Oxide Results: The following results are for the computed nitric oxide levels as functions of engine operating and design variables. Figure 21 shows the exhaust concentration of nitric oxide as functions of the engine load (bmep) for the base case using isooctane and for the

three cases using hydrogen. For isooctane, the nitric oxide values increase as load increases until a bmep of about 700 kPa, and then the nitric oxide concentration remains nearly constant for further load increases. For two hydrogen cases with an equivalence ratio of 1.0, the nitric oxide values increase initially, then level off, and finally, decrease slightly. For the hydrogen case with variable equivalence ratio, the nitric oxide concentration increase, reaches a maximum, and then decreases. This behavior is due to the decrease of equivalence ratio as load decreases. The character of these nitric oxide trends for each of the four cases will be examined next.

Since the nitric oxide kinetics are such strong functions of the gas temperatures, to understand the results in figure 21, the gas temperatures need to be examined. Figures 22–25 show the instantaneous adiabatic zone temperature as functions of crank angle for five engine loads for the three cases, respectively. The temperatures first increase, reach a maximum near the middle of the combustion period, and then decrease during the expansion stroke. The overall temperature comparison shows that the case using hydrogen with fast burn (short burn duration) has the highest temperatures, and the case for isooctane results in the lowest temperatures. As load increases (inlet pressure increases), the gas temperatures increase, but at a decreasing rate due to higher heat losses.

Figures 26–29 show the nitric oxide levels as functions of crank angle (time) for five (5) engine loads for the four cases, respectively. The nitric oxide formation mechanisms dominate shortly after combustion starts. For the cases with the lower temperatures, the nitric oxide concentrations increase, reach a maximum, and remain at that level. For the cases with the highest temperatures, however, the nitric oxide levels reach a maximum, and then begin to decrease due to the decomposition mechanism which is important at the higher temperatures. This decomposition mechanism continues after combustion during the expansion stroke. The computations are terminated when the exhaust valve opens, and the assumption is that no further significant reactions occur.

Figure 21. Nitric oxide emissions as functions of brake mean effective pressure (bmep) for the base case using isooctane and the two cases using hydrogen.

As these results indicate, for sufficiently high temperature cases, the decomposition of nitric oxide can result in lower final concentrations even if the average temperature was higher.

Returning to figure 21, the nitric oxide levels are consistent with the information on the gas temperatures (figures 22–25). The decreasing nitric oxide emissions results for hydrogen can be understood by examining the time-resolved details of these cases. Although generally high gas temperatures result in the highest nitric oxide values, for certain cases with the highest temperatures the decomposition reactions may begin to dominate. This is particularly true for the hydrogen cases for the intermediate and higher loads where the nitric oxide emissions are level or decreasing slightly.

Figure 22. Temperature of adiabatic zone gas as functions of crank angle for five (5) inlet pressures for the base case using isooctane.

Figure 24. Temperature of adiabatic zone gas as functions of crank angle for five (5) inlet pressures for the base case using hydrogen with the 30°CA burn duration.

Figure 23. Temperature of adiabatic zone gas as functions of crank angle for five (5) inlet pressures for the base case using hydrogen with the 60°CA burn duration.

Figure 25. Temperature of adiabatic zone gas as functions of crank angle for five (5) equivalence ratios for the base case using hydrogen with the 30°CA burn duration.

Figure 26. Nitric oxide concentration as functions of crank angle for five (5) inlet pressures for the base case using isooctane.

Figure 28. Nitric oxide concentration as functions of crank angle for five (5) inlet pressures for the base case using hydrogen with the 30°CA burn duration.

Figure 27. Nitric oxide concentration as functions of crank angle for five (5) inlet pressures for the base case using hydrogen with the 60°CA burn duration.

Figure 29. Nitric oxide concentration as functions of crank angle for five (5) equivalence ratios for the base case using hydrogen with the 30°CA burn duration.

Figure 30. Specific nitric oxide emissions as functions of brake mean effective pressure (bmep) for the base case using isooctane and the two cases using hydrogen.

Figure 30 shows the specific nitric oxide emissions as functions of engine load (bmep) for the base case for isooctane, and the two hydrogen cases. For the isooctane case, the specific nitric oxide emissions increase with load, reach a maximum, and then decrease slightly as load increases. On the other hand, the two hydrogen cases have a different trend. For these two cases, the specific nitric oxide emissions are high for low loads, and continue to decrease as load increases. The following will discuss these differences.

The specific nitric oxide emission is related to the nitric oxide concentration via the following relations:

$$\text{spNO} \propto \frac{m_{\text{NO}}}{m_{\text{fuel}}} \times \text{bsfc} \quad 1.$$

$$\text{spNO} \propto \text{NO}_{\text{ppm}} \times \text{bsfc} \quad 2.$$

In other words, the specific nitric oxide emissions are proportional to the nitric oxide concentration and the brake specific fuel consumption. For the hydrogen cases for the conditions considered, the product of the nitric oxide concentration and the brake specific fuel consumption is largest for the low loads and the product continues to decrease as load increases. This is a consequence of

Figure 31. Nitric oxide emission index as functions of brake mean effective pressure (bmep) for the base case using isooctane, and for the two hydrogen cases.

the lower fuel mass of the hydrogen and the higher air-fuel ratio.

One additional way to express the nitric oxide emissions is as an emission index. This is a ratio of the mass of the nitric oxides and fuel consumed. Figure 29 shows the emission index as functions of the engine load for the isooctane case and the two hydrogen cases. For the isooctane case, the emission index increases until about a bmep of 500 kPa, and then remains fairly constant. For the hydrogen cases, the emission index increases rapidly, and then after a maximum has been obtained, the index decreases for additional bmep increases. These results are qualitatively similar to the concentration results shown in figure 21.

SUMMARY AND CONCLUSIONS

This study has used a thermodynamic cycle simulation to investigate the characteristics of using hydrogen (compared to using isooctane) in an automotive, spark-ignition engine. Due to the wide flammability limits and high flame speeds, three cases were examined for using hydrogen: (1) the base case with an equivalence ratio of 1.0 and a burn duration of 60°CA, (2) a case with

an equivalence ratio of 1.0 but with a burn duration of 30°CA, and (3) a case with variable equivalence ratio and a burn duration of 30°CA.

The results included thermal efficiencies, other performance metrics, second law parameters, and nitric oxide emissions:

1. In general, for the cases with an equivalence of 1.0, the brake thermal efficiency was slightly lower for the hydrogen cases due to the higher temperatures and higher heat losses.
2. For the variable, lean equivalence ratio cases, the thermal efficiency was higher for the hydrogen case relative to the isooctane case.
3. Due to the higher temperatures, the hydrogen cases had over 50% higher nitric oxide emissions compared to the isooctane case at the base conditions.
4. The second law analyses indicated that the destruction of availability was lower for the base hydrogen case (11.2%) relative to the isooctane case (21.1%).
5. In general, availability was preserved during the combustion process for the hydrogen cases due to the higher combustion temperatures. This availability was retained in the exhaust gases and the higher temperatures resulted in more availability moved with the heat transfer. The net effect, therefore, was a lower thermal efficiency for the hydrogen cases with an equivalence ratio of 1.0.

Section 3: The Use of Alcohol Fuels

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 the use of methanol resulted in lower entropy production compared to the use of n-dodecane ($\text{n-C}_{12}\text{H}_{26}$). 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 isooctane for part load and full load operation. To accomplish this objective, the study has maintained the same conditions for all fuels.

The following parts of this section of this report include 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 section will end with a brief summary and conclusions.

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.

BASE CASE RESULTS – These first results will include results of cylinder pressure and temperatures, effects of inlet charge temperature, and second law parameters. These results are for the 2000 rpm, and either part load ($\text{bmep} = 325 \text{ kPa}$) or wide open throttle conditions. As described above, 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.

Table 2. Properties of the Fuels [13]

Fuel Vapor	Formula	AF_{stoich}	LHV (MJ/kg _{fuel})
Isooctane	C_8H_{18}	15.07	44.4
Methanol	CH_4O	6.45	20.0
Ethanol	C_2H_6O	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 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.

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 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 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 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%.

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. 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.

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 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 to 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].

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.

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 bmep. 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.

Figure 10. Net indicated thermal efficiency as functions of engine speed for the three fuels for the base case operating conditions.

Figure 9 shows the relative heat transfer (the ratio of the actual heat transfer and the fuel energy input) as functions of engine speed for the three fuels for the base case operating conditions. For these conditions, the relative heat transfer ranges between about 20% and 32% of the fuel input energy. The relative heat transfer decreases as engine speed increases largely due to the shorter available time for the heat transfer (even though the heat transfer coefficient may increase). The three fuels result in nearly the same relative heat transfer.

Figure 10 shows the thermal efficiencies as functions of engine speed for the three fuels for the base case operating conditions. As engine speed increases, the net indicated efficiency (upper portion of the figure) increases largely due to lower relative heat transfer. The alcohol cases have the highest net indicated thermal efficiencies

due to the higher inlet pressures (lower pumping losses; less throttle).

In the lower portion, figure 10 shows the brake thermal efficiency as functions of engine speed for the three fuels for the base case operating conditions. The efficiencies increase from low speeds to about 1900 rpm due to the decreasing importance of the heat transfer (see figure 9). For engine speeds greater than about 1900 rpm, the brake efficiencies decrease due to the increasing importance of mechanical friction. Again, the alcohols achieve higher brake efficiencies due to the lower pumping losses (less throttle) associated with attaining the constant load (bmep) condition.

The brake specific energy consumption as functions of engine speed for the three fuels are essentially the inverse of the brake thermal efficiency curves (figure 11) [22]. The specific energy consumption is a better parameter than the more conventional brake specific fuel consumption (bsfc) since the mass of fuel is less relevant than the energy.

Figures 11 and 12 show the nitric oxide exhaust concentrations as "ppm" and "g/kW-h," respectively, as functions of engine speed for the three fuels for the base case operating conditions. The isooctane case has higher nitric oxide concentrations compared to the alcohol fuels due to slightly higher temperatures. For engine speeds below about 2500 rpm, the nitric oxide concentrations increase for all fuels as engine speed increases due to higher gas temperatures. Figure 13 shows an average adiabatic core temperature as functions of engine speed for the three fuels. The average adiabatic core temperature is the arithmetic time average. Although the gas temperatures were only about 40 K higher for the isooctane case, this is enough of a temperature difference to increase the nitric oxide concentrations. Examining the chemical kinetics associated with nitric oxide formation, a 40 K temperature increase can produce roughly a factor of 1.3 higher nitric oxide concentrations for these conditions which is consistent with the differences in the nitric oxide results.

For engine speeds above about 2500 rpm, the nitric oxide concentrations remain relatively constant. This result for the engine speeds above about 2500 rpm is due mainly to shorter times for the nitric oxide formation. The elapsed time for 90 crank angles is lowered by about half as speed increases from 2500 rpm to 4500 rpm.

To understand some of the above details, instantaneous nitric oxide values were examined at different engine speeds. For example, figure 14 shows the nitric oxide concentrations as functions of crank angle for the 2000 rpm case for the three fuels. Most of the nitric oxide formation occurs during the combustion period for these conditions. By about 60°CA aTDC, the nitric oxide concentrations are essentially “frozen” due to the decreasing temperatures and hence chemical rates.

Figure 15 shows the destruction of exergy during the combustion process as a function of engine speed for the three fuels for the base case operating conditions. The values range from between about 15.5 and 21.5%. The destruction decreases slightly as engine speed increases – this due largely to the higher temperatures. The destruction is higher for isooctane compared to the alcohol fuels – this is largely due to the fundamental nature of the alcohol fuel structure. These are simpler molecules and the entropy production during reaction is lower than for more complex molecules such as isooctane. Similar conclusions for the combustion of alcohol fuels have been reported by others (e.g., [8]).

Figure 11. Nitric oxide emissions as functions of engine speed for the three fuels for the base case operating conditions.

Figure 12. Specific nitric oxide emissions as functions of engine speed for the three fuels for the base case operating conditions.

Figure 13. Average adiabatic-zone temperatures as functions of engine speed for the three fuels for the base case operating conditions.

Figure 14. Nitric oxide concentrations and adiabatic flame temperatures as functions of crank angle for the three fuels for the base case operating conditions at 2000 rpm.

Figure 15. Destruction of exergy during the combustion process (as a percentage of the fuel exergy) as functions of engine speed for the three fuels for the base case operating conditions.

EFFECTS OF ENGINE LOAD – The next set of results reflect the engine performance and characteristics as functions of engine load (bmep) for a constant engine speed of 2000 rpm for an equivalence ratio of 1.0 and MBT timing.

The inlet pressures increase linearly as load increases, and as described above, the alcohol fuels operate with a slightly higher inlet pressure (less throttle; less pumping losses) for the same load (bmep). The higher inlet pressures are needed to compensate for the higher fraction of fuel vapor for the alcohols compared to isooctane which displaces air.

Figure 16 shows the net **indicated** thermal efficiency as functions of engine load for the three fuels for the base case operating conditions. The efficiencies increase as engine load increases largely due to the reduction in pumping losses. The two alcohol fuels have slightly higher thermal efficiencies than the isooctane case since they are operating at slightly higher inlet pressures (less throttle) for the same load.

Figure 16 also shows the **brake** thermal efficiency as functions of engine load for the three fuels for the base case operating conditions. The brake efficiencies are slightly less than the indicated efficiencies due largely to cylinder heat transfer and mechanical friction.

Figure 16. Net indicated and brake thermal efficiencies as functions of engine load (bmep) for the three fuels for the base case operating conditions.

Figure 18. Enthalpy-averaged exhaust temperatures as functions of engine load (bmep) for the three fuels for the base case operating conditions.

Figure 17. Relative heat transfer (energy) as functions of engine load (bmep) for the base conditions for the three fuels.

Figure 19. Nitric oxide concentrations as functions of engine load (bmep) for the three fuels for the base case operating conditions.

Figure 20. Specific nitric oxide concentrations as functions of engine load (bmep) for the three fuels for the base case operating conditions.

Figure 22. Exhaust energy (top) and exergy (bottom) as functions of engine load (bmep) for the base conditions for the three fuels.

Figure 21. Average combustion temperature as functions of engine load (bmep) for the base conditions for the three fuels.

Figure 23. Heat transfer exergy as functions of engine load (bmep) for the base conditions for the three fuels.

Figure 24. Exergy destroyed during the combustion process as a percentage of the input fuel exergy as functions of engine load (bmep) for the base conditions for the three fuels.

Figure 17 shows the relative heat transfer (percentage of inlet fuel energy) as functions of engine load for the three fuels for the base case operating conditions. The relative heat transfer is similar (between about 20% and 45%) for each fuel and decreases rapidly with increases in engine load. Although the absolute heat transfer increases with engine load (due largely to higher temperatures), the inlet fuel energy increases more rapidly.

Figure 18 shows the enthalpy-averaged exhaust gas temperatures as functions of engine load for the three fuels for the base case operating conditions. The exhaust temperature increases from about 1200 K to about 1300 K as load increases from idle to full load for these conditions. The alcohol fuels result in slightly lower exhaust temperatures. Due to the conditions of these computations, the gas temperatures are not dramatically different for the three fuels. These conditions include the fact that the fuel vaporization occurs outside the engine cylinder and does not change the inlet temperature. In addition, the cylinder wall temperatures are assumed the same for all fuels.

Figures 19 and 20 show the nitric oxide concentrations as “ppm” and “g/kW-h,” respectively, as functions of load for the three fuels for the base case operating conditions. In figure 19, the nitric oxide concentrations increase from about 500 ppm to over 3000 ppm as load increases from idle to full load for these conditions. The alcohol fuels have slightly lower values throughout the load range. These lower values are due to the slightly lower gas temperatures as described previously (and below with figure 21). The specific nitric oxide concentrations (figure 20) increase from idle to about mid-load and then decrease slightly for further increases of load.

Figure 21 shows the average combustion gas temperatures as functions of engine load for the three fuels for the base case operating conditions. The average combustion gas temperature is the average one-zone temperature during the combustion duration. The combustion temperature increases as load increases – this is a reason for the nitric oxide results.

Figure 22 shows the exhaust gas energy (top) and exergy (bottom) as percentages of the input energy and exergy, respectively, as functions of engine load for the three fuels for the base case operating conditions. The exhaust energy and exergy increase from idle to about a bmep of 300 kPa, and then remain fairly constant for further increases of load. This is partly the result of the exhaust gas temperature (figure 18). As described above, the specific exergy values are based on the internal energy, specific volume, pressure, entropy and dead state values. This results in the exergy values depending not only on the temperature but on the pressure and the relation of the other thermodynamic properties to these quantities.

Figure 23 shows the heat transfer exergy as a percentage of the inlet fuel exergy as functions of engine load for the three fuels for the base case operating conditions. These values range from about 16% to 34% for these conditions, and the three fuels result in similar values (compare to figure 17 which shows the related values based on energy).

Figure 24 shows the exergy destroyed during the combustion process as a percentage of the inlet fuel exergy as functions of load for the three fuels for the base case operating conditions. The exergy destroyed is not a strong function of load, and is highest for isooctane and lowest for ethanol. This is similar to the above results in

figure 15 which showed the exergy destroyed as a function of speed.

Conclusions: A thermodynamic engine cycle simulation was used to examine the use of alcohol fuels (methanol and ethanol) in an automotive, spark-ignition engine from a first and second law perspective. Results were obtained for a constant load (bmep) condition as functions of engine speed, and for a constant speed as functions of engine load. Spark timing was determined for maximum bmep, and the equivalence ratio was 1.0. All cases were based on completely vaporized fuel uniformly mixed with the incoming air, constant inlet temperature, and the same cylinder wall temperature.

1. Although the alcohol fuels have only about one-half of the heating value of isooctane per unit (mass or volume), the input fuel energy of the stoichiometric mixtures for the alcohol fuels are only slightly (<3%) lower than for isooctane.

2. To attain the same load, the inlet pressure of the alcohol fuels needed to be slightly higher (less throttle).

These higher inlet pressures compensate for the higher fraction of fuel vapor for the alcohol fuels which displaces air and lowers the fuel energy density.

3. For the conditions of this study, the heat transfer was about the same for all fuels. These conditions included the same inlet temperature, premixed mixtures, and constant wall temperatures.

4. The indicated and brake thermal efficiencies were slightly higher for the alcohol fuels compared to isooctane due to the lower pumping losses (less throttle). Higher inlet pressures (less throttle) were needed to obtain the same load for the alcohol fuels to compensate for the larger amount of fuel vapor (which displaced air).

5. Nitric oxide concentrations for isooctane were higher than for the alcohol fuels due to the slightly higher gas temperatures during combustion.

6. Destruction of the fuel exergy during the combustion process was higher for isooctane compared to the alcohol fuels due to the more complex molecular structure of the isooctane fuel.

Section 4: Compression Ratio and Expansion Ratio

The importance of compression ratio and expansion ratio for conventional, reciprocating, internal combustion engines has been recognized from the very beginning of engine development. A large literature exists for both experimental and analytical results as functions of compression ratio and, to a lesser extent, of expansion ratio. Increases of the compression ratio and expansion ratio are known to increase the thermodynamic advantages, but these gains are often limited by knock. The current work is a detailed study of the effects of compression ratio and expansion ratio on engine performance from both a first law and second law perspective.

An important feature of the current work is to examine the effects of the expansion ratio independent of the compression ratio. This arrangement will be described in more detail below, but in general, this is often called an Atkinson cycle. The actual mechanism will not be the focus, but rather, the benefits of such arrangements from a thermodynamic view point. A wide range of conditions will be examined including part load and full load operation.

The following parts of this section will include a brief review of previous work, a description of the engine and operating conditions, and a presentation of the results. The results will be divided into three sections: (1) compression ratio effects, (2) expansion ratio effects for part throttle, and (3) expansion ratio effects for wide open throttle. Finally, this section will end with a summary and conclusions.

Previous Work: This section will provide a brief summary of some of the previous work in this area. Investigations of engine performance as a function of compression ratio have a long history. An early, classical paper by Caris and Nelson [1] is often cited with respect to the importance of compression ratio for spark-ignited engines. By using special fuels and fuel additives, spark knocking was avoided even for the highest compression ratios tested. They demonstrated maximum performance for a specific compression ratio, and for greater compression ratios the performance remained constant or decreased slightly. Another useful reference is the work by Muranaka, et al. [2]. They reported experimental results and provided explanations for the improvement in performance for increases in compression ratio. They found that the items that limit the improvement of thermal efficiency as compression ratio increase were increased heat transfer and

incomplete or slow burning. They stated that the effect of combustion duration changes with compression ratio changes was minor.

For a conventional, four-stroke cycle, spark-ignited engine, the compression and expansion strokes are equal. The gases at the end of a conventional expansion process, however, possess the potential to produce more work if allowed to expand to a greater volume. By the use of special linkages, the expansion ratio could be greater than the compression ratio, and thereby, provide the potential for greater overall thermodynamic gains. This concept, originally patented [3] in the mid 1880s by James Atkinson, a British engineer, is known as the Atkinson cycle or (in a generic sense) an over-expanded cycle.

Another concept that is closely related is often called the Miller cycle [4], and involves using either early or late intake valve closing to reduce the effective compression ratio relative to the expansion ratio. This concept has been relatively successful and exists in a number of commercial engines (e.g., [5]). Although the Atkinson and Miller cycles are related, they possess unique features. For example, the Miller cycle with late intake valve closing will move gases into the intake system during the initial period of the compression stroke. Also, some studies have shown that certain timings of the intake valve closing cause poor combustion [6]. The Atkinson cycle, on the other hand, can independently optimize valve events. The Atkinson cycle, however, will require a more complex mechanism and incur additional frictional losses.

Previous studies of the Atkinson and Miller cycles are numerous (e.g., [7–10]). Most of these studies are based on the Miller cycle; only a few are based on mechanical features which provide a longer expansion stroke relative to the compression stroke (e.g., [11]).

RESULTS AND DISCUSSION

This study was divided into two major parts: (1) a study of the effects of compression ratio (with an equal expansion ratio), and (2) a study of the effects of the expansion ratio (where the compression ratio was smaller and constant).

Study Constraints: The following results are based on a set of assumptions and approximations which did not consider all features. For example, combustion stability, cycle-to-cycle variations, or other combustion issues are not included. In addition, knock, preignition, or other abnormal combustion phenomena are not considered. In addition, mechanical friction was based on conventional engines (further comments on friction are described below). Due to these assumptions and approximations, the following results may be optimistic.

Compression Ratio: Figures 2–4 show the resulting cylinder pressures and (spatial) average gas temperatures as functions of crank angle for compression ratios of 6, 10, 16 and 20 for the base case part load condition. To maintain the constant load (bmep = 325 kPa), the inlet pressure is adjusted. For example, for increases of compression ratio, the inlet pressure decreases. This difference of the inlet pressure is not noticeable on the scale of the figure. The cylinder pressures increase directly as compression ratio increases. Peak cylinder pressures almost double as compression ratios increased from 6 to 20. In contrast, the peak cylinder gas temperatures were highest for the lower compression ratios. During the compression stroke, the cylinder gas temperature increases most for the higher compression ratios. During the combustion period, however, the gas temperature increases most for the lower compression ratios. During the expansion stroke, the temperatures remain highest for the lower compression ratio cases. These higher temperatures for the lower compression ratio cases are due to slightly lower heat transfer, lower thermal efficiency, and less efficient expansion.

Figure 5 shows the time-average cylinder gas temperature during the combustion period as functions of compression ratio for both part load (bmep = 325 kPa) and wide open throttle (WOT). This temperature first increases, reaches a maximum for a compression ratio of about 8 and then decreases as compression ratio increases. These temperature changes, however, are relatively modest: for the part load case, the total temperature

change for the average cylinder gas temperature during the combustion period for the range of compression ratios examined was less than 5%.

The average cylinder gas temperature during the combustion period is the net result of several items. The first item is the starting temperature (the temperature at the end of compression). This item results in higher temperatures as compression ratio increases. The other items all tend to decrease the gas temperature. These items are the slight increase in heat transfer (due to higher heat transfer coefficients, see below), higher thermal efficiencies, and the more efficient expansion process as compression ratio increases. The net result of these items on the gas temperature appear to be about balanced for a compression ratio of about 8 for the conditions studied.

Figure 2. Cylinder pressures as functions of crank angle for compression ratios of 6, 10, 16 and 20.

Figure 3. Cylinder temperatures as functions of crank angle for compression ratios of 6, 10, 16 and 20.

Figure 4. Cylinder temperatures near TDC as functions of crank angle for compression ratios of 6, 10, 16 and 20.

Figure 5. Average cylinder temperatures during the combustion period as functions of compression ratio for both part load and WOT cases.

Figure 6. Indicated thermal efficiencies as functions of compression ratio for two ideal "Otto" cycles, for a part load (bmep = 325 kPa) case, and for a WOT case.

Figure 7. Indicated and brake thermal efficiencies as functions of compression ratio for the part load (bmep = 325 kPa) case.

Figure 8. Instantaneous heat transfer coefficient as functions of crank angle for compression ratios of 6, 10, 16 and 20.

Figure 6 shows the indicated thermal efficiencies as functions of compression ratio for ideal “Otto” cycles and for two simulation cases (part load and WOT). The ideal “Otto” cycle efficiency results are based on the simple relation:

$$\eta = 1 - r^{(1-k)} \quad 1.$$

where r is the compression ratio and k is the ratio of specific heats. The ratio of the specific heats, k , was selected to be either 1.4 (cold) or 1.3 (hot). These values span the typical range expected for most operating conditions. Recall that the ideal “Otto” cycle efficiency is derived for adiabatic processes with instantaneous heat addition at TDC, with no mechanical or fluid friction, and no flows. The other two curves in this figure represent the net indicated thermal efficiencies from the simulation for the part load (bmep = 325 kPa) and wide open throttle (WOT) cases. In general, the thermal efficiency increases with increases of compression ratio. The greatest increases are for the initial compression ratio increases up to about 10. The thermal efficiency continues to increase for further increases in compression ratio, but the gains are less and less. Relative to the simulation results, the ideal results are roughly 50% too high. A major part of the difference between the ideal and simulation results is the assumption of adiabatic processes for the ideal calculations. In addition, the lack of flow processes, the instantaneous heat addition, and the constant property assumption contribute to the overprediction of thermal efficiency.

Figure 7 shows the brake and indicated thermal efficiencies as functions of compression ratio for the part load case. These efficiencies increase rapidly at first, and then with a lower rate of increase as compression ratio increases.

The relative importance of cylinder heat transfer is examined next. The cylinder heat transfer is related to the surface area (A_{surf}), the heat transfer coefficient (h_{heat}), and the temperature difference between the gas and the cylinder walls (ΔT):

$$\dot{Q} \propto A_{surf} h_{heat} \Delta T \quad \bullet$$

The surface area decreases slightly for increasing compression ratio, and as shown in figure 5, the temperature difference first increases and then decreases for increasing compression ratios (but these are modest changes).

Figure 8 shows the instantaneous heat transfer coefficient as functions of crank angle for compression ratios of 6, 10, 16 and 20. The heat transfer coefficient increases with increasing compression ratio. For an increase of compression ratio from 6 to 20, the peak heat transfer coefficient almost triples in value. The net result of these items is a slight increase in the heat transfer as compression ratio increases. Figure 9 shows the relative heat transfer and relative net exhaust energy as functions of compression ratio for the part load case. The “relative” values are the actual values divided by the fueling rate. As compression ratio increases, the thermal efficiency and the heat transfer increases, and this results in a decrease in the net exhaust energy.

Figure 9. Relative net exhaust energy and relative heat transfer as functions of compression ratio for the part load case.

Figure 10. Relative energy values as functions of compression ratio for the part load case.

Figure 11. Availability destroyed during the combustion process as functions of compression ratio for the part load case and wide open throttle cases.

Figure 12. Relative availability values as functions of compression ratio for the part load case.

Figure 10 shows the distribution of the fuel energy between work, heat transfer and exhaust as functions of compression ratio. Brake and indicated work increase as compression ratio increases (similar to figure 7). Also shown is the slight increase in friction work due to the increase in compression ratio. The heat transfer fraction increases and the net exhaust energy fraction decreases as compression ratio increases. Finally, at the top of the figure, a small amount (0.7%) of the fuel energy is unburned.

Figure 11 shows the availability destroyed during the combustion process as functions of compression ratio for the part load and wide open throttle cases. The availability destroyed decreases from about 23% to about 21% for the part load case as the compression ratio increases from 4 to 10. For increases of compression ratio from 10 to 20, the availability destroyed is nearly constant. The wide open throttle case results in slightly less availability destroyed for the higher compression ratios.

The results of figure 11 are largely a result of temperature and pressure changes. As shown in figure 5, the average gas temperature during the combustion process increases for compression ratio increases from 2

to 8. This is, at least, a part of the reason for the decrease in the availability destruction for this range of compression ratios. For the compression ratio range of 8 to 20, the temperature decrease (figure 5) is off-set by the pressure increases such that the destruction of availability decreases slightly.

Finally, figure 12 shows the distribution of the relative availability as a function of compression ratio for the part load case. The following is a description of these results from the bottom to the top of the figure. Again, the indicated work increases as compression ratio increases, and this is similar to figure 7. The next item is the availability moved with the heat transfer which increases as compression ratio increases. The increase of the heat transfer as compression ratio increases is described above. The net availability that leaves with the exhaust gases decreases as compression ratio increases. The availability destroyed during the combustion process only slightly decreases as compression ratio increases. The availability destroyed as the incoming fuel-air mixture mixes with the residual gases decreases as compression ratio increases. This is largely a result of the high residual fractions associated with the lower compression ratio cases. Finally, at the top, is the availability associated with the unburned fuel.

These results were for compression ratios up to 20. Higher compression ratios were briefly examined. The trends were maintained for a compression ratio of 40, and no particular advantage was observed. The trend to lower combustion temperatures continued. For example, for a compression ratio of 40 for the part load case, the average gas temperature during combustion was 1550 K, and the availability destroyed during the combustion process was 21.4%.

Expansion Ratio – Part Load: In the above, a conventional engine was examined which had the same compression ratio and expansion ratio. Since the expansion ratio is expected to be more important than the compression ratio in terms of thermodynamic work production, an Atkinson cycle was examined next. To study the Atkinson cycle, a number of approaches may be considered. The current study has adopted the following set of assumptions and approximations:

- The piston motion will be assumed to be approximated by two superimposed motions based on the classic “slider-crank” mechanism.

- The clearance volume will be based on the compression ratio (CR) and the stroke dimension (S_{comp}) of the standard engine.
- By selecting an expansion ratio (ER) and using the clearance volume from above, the expansion stroke (S_{exp}) can be determined.
- The transition between the compression and expansion strokes will be at 0.0°CA (TDC during combustion) and 360°aTDC.
- The engine mechanical friction will be based on the standard engine using the compression ratio. The slight increase of friction due to the longer expansion stroke will be neglected. (The effect of other friction assumptions are considered at the end of the results section.)
- The engine performance parameters (such as bmep) will be based on the standard engine configuration using the compression stroke to determine the displaced volume.
- As mentioned above, items such as knock, preignition, roughness, and cyclic variability are ignored for this preliminary study.

First, some of the required variables will be defined. The compression ratio follows the normal definition:

$$CR = \frac{V_{comp}}{V_{cl}} \quad \bullet$$

where V_{comp} is the total cylinder volume based on the compression stroke length (S_{comp}) and V_{cl} is the clearance volume. The expansion ratio is

$$ER = \frac{V_{exp}}{V_{cl}} \quad \bullet$$

where V_{exp} is the total cylinder volume based on the expansion stroke length (S_{exp}). The “displaced” volumes are

$$V_{disp,compression} = \frac{\pi B^2}{4} S_{comp} \quad \bullet$$

$$V_{disp,expansion} = \frac{\pi B^2}{4} S_{expansion} \quad \bullet$$

A multiplier factor for the expansion stroke relative to the compression stroke may also be defined

$$\frac{S_{exp}}{S_{comp}} = \frac{ER}{CR} = \text{Stroke Multiplier} \quad \bullet$$

For example, if an expansion ratio of 15 is desired and the compression ratio is 10, then the expansion stroke must be increased by a factor of 1.5 relative to the compression stroke.

The first example of results for the Atkinson cycle is based on a compression ratio of 15 and an expansion ratio of 20. Figure 13 shows the instantaneous cylinder volume as a function of crank angle for this configuration, and for reference, also shows the cylinder volume for the conventional case where the compression ratio and expansion ratio are the same (and equal to 15). To the right of the figure is a schematic of the cylinder arrangement with the two stroke dimensions indicated. The cylinder volume decreases during the compression stroke from intake valve close (IVC) to TDC (0.0°CA), then increases to a maximum volume during the expansion stroke from TDC to 180°aTDC. Although two expressions were used for the volume computation, the transition appears smooth on this scale.

Figure 14 shows the related change of volume as functions of crank angle for the above case for a compression ratio of 15 and an expansion ratio of 20. Again, for reference, the change of volume is also shown for the conventional case where the compression ratio and expansion ratio are the same (and equal to 15). Also again, the transition between the two expressions appears smooth. For other cases with greater differences between the compression ratio and expansion ratio (say, CR = 6 and ER = 30), the transitions were not as smooth.

Figure 15 shows the computed brake thermal efficiency as functions of expansion ratio for three compression ratios (6, 10 and 15) for the base case part load engine conditions. For these computations, the bmep was constant (= 325 kPa) – so as the brake efficiency increased, the inlet pressure was reduced. For each compression ratio case, as the expansion ratio increases the thermal efficiency first increases, reaches a maximum, and then decreases. The expansion ratio for the highest efficiency appears to be equal to about the compression ratio plus three. The use of this expansion ratio provides a thermal

efficiency increase of about 1% (e.g., from 24% to 25%). These results are examined more fully in the following.

Figure 13. Cylinder volume as a function of crank angle for a compression ratio of 15 and for expansion ratios of 15 (dashed lines) and 20 (solid lines). Schematic of engine cylinder shown on right side.

Figure 14. Rate of change of volume as functions of crank angle for a compression ratio of 15 and for expansion ratios of 15 (dashed lines) and 20 (solid lines).

Figure 15. Brake thermal efficiency as functions of the expansion ratio for the base case for three compression ratios.

First, the case with a compression ratio of 15 and an expansion ratio of 20 (solid lines) will be examined. This case represents the highest efficiencies of the cases examined. Figure 16 shows the log of the cylinder pressure as functions of the log of the cylinder volume. The conventional case (dashed lines) with $CR=ER=15$ is compared with the case with an expansion ratio of 20 (solid lines). The longer expansion stroke results in a maximum cylinder volume of about 0.973 dm^3 , while the conventional case has a maximum cylinder volume of 0.717 dm^3 . The inlet pressure is slightly lower for the over expanded case, and this results in generally lower pressures throughout most of the cycle.

Figure 17 shows the log of the one-zone, cylinder gas temperature as functions of the log of the cylinder volume for the base case conditions for a compression ratio of 15 and an expansion ratio of 20 (solid lines), and for the conventional case ($CR=ER=15$; dashed lines). Denoted on this figure by circles are the various events (such as EVO, EVC, ...). Starting with the intake valve closing (IVC), the temperature increases during the compression stroke and during the combustion process. After the majority of the expansion stroke, the exhaust valve opens

(EVO) at 116°aTDC , and after BDC, the temperature decreases during the exhaust stroke. The two cases have similar temperatures, but the overexpanded case has slightly higher temperatures for most of the cycle.

Figure 18 shows the intake and exhaust flow rates as functions of crank angle for the two cases. The most significant difference is the lower flow rates during the blow-down portion of the exhaust flow for the overexpanded cases. This is because of the greater expansion which results in a lower cylinder pressure at the time of exhaust valve opening. This is compensated by the greater flow rates during the exhaust displacement phase of the exhaust process. The effect of the exhaust valve open time is examined below.

The next item to discuss is the results in figure 15 which indicated that for each compression ratio a specific expansion ratio provided the maximum efficiency. This will be examined for the case with a compression ratio of 6.0. Figure 19 shows the relative energy distribution (based on the lower heating value of the fuel) for this compression ratio of 6.0 as functions of the expansion ratio. The brake work percentages are equivalent to the earlier shown brake thermal efficiencies. The relative heat transfer increases as expansion ratio increases. This is largely due to the increase of surface area as the expansion ratio increases. The relative energy leaving in the exhaust first decreases, and then increases slightly for the expansion ratios greater than about 12. This is a net result of the energy delivered as work and transferred out of the system via heat transfer. For the higher expansion ratios, the work is decreasing faster than the heat transfer is increasing, and this results in a net increase of the exhaust energy.

Figure 16. Log of the cylinder gas pressure as functions of the log of the cylinder volume for the base case for a compression ratio of 15 and for expansion ratios of 15 (dashed lines) and 20 (solid lines).

Figure 17. Log of the one-zone, cylinder gas temperature as functions of the log of the cylinder volume for the base case for a compression ratio of 15 and for expansion ratios of 15 (dashed lines) and 20 (solid lines).

Figure 18. Exhaust and intake flow rates as functions of crank angle for the base case for a compression ratio of 15 and for expansion ratios of 15 (dashed lines) and 20 (solid lines).

Figure 19. Relative energy as functions of the expansion ratio for the base case for a compression ratio of 6.

Figure 20. Log of the cylinder gas pressure as functions of the log of the cylinder volume for the base case for a compression ratio of 6 and expansion ratios of 8 and 10.

Figure 21. Exhaust and intake flow rates as functions of crank angle for the base case for a compression ratio of 6 for two expansion ratios: (1) optimum, ER = 8, and (2) not optimum, ER = 10.

Figure 22. Log of the cylinder gas pressure as functions of the log of the cylinder volume for the base case for a compression ratio of 6 and an expansion ratio of 10 for two different exhaust valve open timings.

The cases which will be examined in some detail are for expansion ratios of 8 (near maximum efficiency) and 10 (both for a compression ratio of 6). The question is why does the thermal efficiency begin to decrease even as the expansion ratio increases from 8 to 10. Figure 20 shows the log pressure as a function of the log volume for these two cases. These results are similar to those in figure 16. Also shown on this figure is the location of the exhaust valve open (EVO) event. Due to the longer expansion stroke, this occurs at a lower pressure for the case with an expansion ratio of 10. Figure 21 shows the intake and exhaust flow rates as functions of crank angle for the two cases. As shown above (figure 18), the most significant difference is the much lower flow rates during the blowdown portion for the case with an expansion ratio of 10. In fact, for expansion ratios higher than 10, due to the low cylinder pressures, the initial blowdown is back into the cylinder (rather than out of the cylinder). The lack of an effective exhaust blowdown for higher expansion ratios is one of the reasons that the higher expansion ratios result in decreasing efficiencies.

Since the timing of the exhaust valve opening may be important, this was examined as well. Figure 22 shows the log of the cylinder pressure as a function of the log of the cylinder volume for the case with a compression ratio of 6 and an expansion ratio of 10 for two EVO timings: an early opening at 96°aTDC and a late opening at 146°aTDC. The cylinder pressures and thermal efficiencies are nearly the same for these changes of the EVO.

Figure 23. Brake thermal efficiency as a function of expansion ratio for compression ratios of 6, 10 and 15 for an engine speed of 1400 rpm and an inlet manifold pressure of 95 kPa (WOT).

Figure 24. Log of cylinder pressure as a function of log of cylinder volume for a compression ratio of 15 and expansion ratios of 15 and 44 for an engine speed of 1400 rpm and an inlet manifold pressure of 95 kPa (WOT).

Figure 25. Ratio of brake thermal efficiencies as a function of the ratio of the expansion stroke length and compression stroke length for a compression ratio of 15 for an engine speed of 1400 rpm and an inlet manifold pressure of 95 kPa (WOT).

Figure 26. Mass flow rates as a function of crank angle for a compression ratio of 15 and two expansion ratios (15 and 44) for an engine speed of 1400 rpm and an inlet manifold pressure of 95 kPa (WOT).

Figure 27. Availability destruction due to combustion as a function of the expansion ratio for a compression ratio of 15 for an engine speed of 1400 rpm and an inlet manifold pressure of 95 kPa (WOT).

Finally, the destruction of availability during the combustion process as a function of expansion ratio was examined. For the case with a compression ratio of 6, the percentage of availability destroyed was nearly constant, and ranged between 21.74% and 21.79% for expansion ratios between 6 and 14. One of the major reasons for this negligible difference is the modest changes of the combustion gas temperatures as the expansion ratio increased.

Expansion Ratio – WOT: In addition to the above results for a part load condition, results were obtained for the use of greater expansion ratios for the case of wide open throttle. Figure 23 shows the brake thermal efficiency as functions of the expansion ratio for three compression ratios (6, 10 and 15). For each compression ratio, the thermal efficiency first increases, reaches a maximum, and then decreases. The expansion ratio for the highest thermal efficiency is about 19, 29, and 44 for the compression ratios of 6, 10 and 15, respectively. The use of these expansion ratios resulted in an increase of the thermal efficiency of about 10%. For example, for a compression ratio of 6, the brake thermal efficiency increased from about 30% to slightly over 40% as the expansion ratio increases from 6 to about 19. Compared to the previous part load cases, the WOT cases result in much greater improvements with greater values of expansion ratios. The following will discuss some aspects of these results.

Figure 24 shows the log of the cylinder pressure as a function of the log of the cylinder volume for the WOT case with the highest brake thermal efficiency (of the cases examined) which was for a compression ratio of 15 and an expansion ratio of 44 (solid line). For comparison, figure 24 also shows (dashed line) the results for the WOT case for a compression ratio of 15 and an expansion ratio of 15 (standard engine configuration). The pressures during the compression stroke are the same for both configurations, but the pressures during the expansion are different, and of course, for the over-expanded configuration, the expansion proceeds to a much greater volume. The additional area within the pressure-volume diagram associated with the over-expanded configuration is indicative of the additional work (power) obtained with the greater expansion. The pressures for the exhaust stroke are generally higher for the over-expanded configuration, but the pressures during the intake stroke are nearly the same.

Figure 25 shows the relative increase in the brake thermal efficiency as a function of the increase of the length of the expansion stroke relative to the length of the compression stroke for the case with a compression stroke of 15. As an example, the expansion stroke length must increase about 3 times the compression stroke length to achieve the highest thermal efficiency for the conditions examined. This could be impractical for the modest gains.

Figure 26 shows the mass flows as functions of crank angle for two cases. For the standard configuration, the blowdown portion of the exhaust flow is significant whereas for the over-expanded case, the blow-down portion is much less significant. For the over-expanded case, the majority of the exhaust flow occurs during the displacement portion of the exhaust flow. In addition, for the over-expanded case, the back-flow after the blowdown is much more significant. For expansion ratios greater than about 44 (not shown), the exhaust process is compromised, and when the exhaust valve first opens, the flow is back into the cylinder. The intake flows are nearly the same for both configurations.

For completeness, figure 27 shows that the availability destroyed due to combustion increases slightly (from about 20.2% to 21.0%) as the expansion ratio increases from 15 to 55 for a compression ratio of 15 for the WOT case. This slight increase is due to the lower combustion temperatures associated with the higher expansion cases. Since the work output increases for the higher expansion ratios, the gas temperatures decrease which is a major cause of availability destruction during the combustion process [13].

One final consideration was the mechanical friction. For an over-expanded configuration, the mechanical friction would be expected to be higher due to the additional mechanism and the longer stroke. This can not be quantified without some knowledge of the specific design and experimental information. To explore this issue, some estimates were completed. By assuming that the friction was due to an engine configuration possessing the expansion ratio for both the compression and expansion strokes (a higher estimate for the friction component), the maximum thermal efficiency decreased by about 2% (i.e., from 45% to 43%). In addition, the optimum expansion ratio for the higher friction case decreased. Again, a more

detailed consideration of friction would be needed for a particular mechanism.

Conclusions: This section has presented results for the effects of compression ratio and expansion ratio on performance, efficiency, and second law parameters for an automotive, spark-ignition engine. The cases with greater expansion ratios than compression ratios are often called “Atkinson” cycles. For these cases, the expansion ratio was assumed independent of the compression ratio. The results of this study may be summarized as follows:

- Indicated and brake performance increase for increases in compression ratio. These gains are most significant up to a compression ratio of about 10.
- For the highest compression ratios (>10), gains of brake performance and efficiency with further compression ratio increases are modest for the conditions studied. The results demonstrated that the increasing friction and heat losses for the higher compression ratios are of the same order as the thermodynamic gains.
- For the part load condition, the availability destroyed due to the combustion process decreased from about 23% for a compression ratio of 4 to about 21% for a compression ratio of 10.
- The study included expansion ratios up to four (4) times the compression ratio. For most cases, the thermal efficiency first increased as expansion ratio increased, then attained a maximum efficiency, and then decreased. The decrease in efficiency after the maximum value was shown to be due to increased heat losses, increased friction, and ineffective exhaust processes (due to the reduced cylinder pressure at the time of exhaust valve opening).
- For the part load cases, the higher expansion ratio provided only modest gains due to increased pumping losses associated with the constant load requirement.
- For the wide open throttle cases, however, the higher expansion ratios provided significant gains. For example, for a compression ratio of 10, expansion ratios of 10 and 30 provided brake thermal efficiencies of about 34% and 43%, respectively. Although the net thermodynamic gains are significant, large expansion ratios such as 30 may not be practical for most applications.
- For the wide open throttle cases, for a compression ratio of 15, the availability destroyed due to the combustion process increased slightly from about 20.2% to 21.0% as the expansion ratio increased from 15 to 55.

Section 5: The Use of Turbocharging

The use of turbocharging systems for spark-ignition engines has seen increased interest in recent years due to the importance of fuel efficiency, and in some cases, increased performance. Current spark ignition engines with turbocharging systems are typically operated near stoichiometric with three-way catalyst systems and exhaust gas recirculation for low emissions. Other operating modes include lean overall stoichiometry to avoid knock and improve efficiency.

The major advantage of turbocharging is attaining higher specific power compared to naturally aspirated engines. This may allow smaller engines with their better packaging characteristics for the same application. For full load operation, a turbocharged engine may be able to demonstrate higher thermal efficiencies compared to a naturally aspirated engine.

Some of the noted disadvantages when using turbocharging include the increased propensity for knock, the requirement of higher octane fuels, and possibly higher maintenance. For some applications, the engine may lack responsiveness ("lag"), and may suffer abrupt power surges as the turbocharger is engaged. Finally, turbocharged engines are more costly and complex.

The purpose of the current work is to quantify the effects of turbocharging with respect to the first law and second law of thermodynamics. In particular, the relative importance of the various components on the overall performance characteristics of the engine system will be determined.

Previous Work: Few investigations have focused on the use of the second law of thermodynamics to better understand the use of turbocharging for spark-ignition engines. A much larger set of literature exists regarding the use of turbocharging for compression ignition (diesel) engines. Previous work based on compression ignition engines is outside the scope of this work. The following, therefore, are examples of some of the literature concerning turbocharging and spark-ignition engines.

Watts and Heywood [3] in 1980 published a fairly complete assessment of a turbocharged spark-ignition engine using a thermodynamic simulation. Their work did not include the second law of thermodynamics, but they did complete a fairly detailed study including a compari-

son with a larger (5.7 liter), naturally aspirated engine. Some elements of this study [3] have been adopted here. In general, they found that the 3.8 liter turbocharged engine was more efficient than the 5.7 liter, naturally aspirated engine for typical vehicle operating conditions. The 3.8 liter turbocharged engine generally operated at higher temperatures and pressures.

In work related to the second law aspects (but based on a diesel engine), Bozza et al. [4] in 1991 used the second law of thermodynamics to investigate turbocharged engine operation. They found that in general turbocharging could not be considered an effective method for availability recovery. They reported that the losses associated with the turbocharger components are only partially compensated for by the slight reduction in the combustion irreversibilities.

Filipi and Assanis [5] in 1991 reported the results of an investigation using a quasi-dimensional engine cycle simulation to examine a four-cylinder, turbocharged, spark ignition engine. Among other items, they examined the advantages of a four or two valve (per cylinder) engine design. They did not employ any second law considerations.

Duchaussoy et al. [6] in 2003 studied the dilution aspects associated with a turbocharged spark-ignition engine at full load. They completed an experimental and analytical study which compared lean operation with the use of EGR. They found advantages of the use of EGR relative to lean operation. They noted a reduction of knock tendencies and improved efficiencies.

In 2007, Bozza et al. [7] published results for a turbocharged spark ignition engine using a commercial engine cycle simulation. They reported both steady state and transient results. They did not use the second law of thermodynamics.

Li and Karim [8] in 2008 published results from simulation studies concerning a turbocharged engine operating with natural gas. They did not report on any second law considerations. The emphasis of their work was the use of hot EGR and implications on knock. They reported that the application of hot EGR increased the tendency for knock, but that the use of EGR also increased the knock limited boost pressure ratio. They examined strategies for effectively using EGR for their conditions.

Figure 2. A schematic of the complete engine system including the compressor, intercooler and turbine.

Finally, in 2008, Rakopoulos and Michos [9] have published one of the few studies of a turbocharged spark-ignition engine which was based in part on the second law of thermodynamics. In this work, they used only the closed cycle, so estimates were needed for the initial conditions (e.g., residual gas, temperature and pressure). Their emphasis was on the combustion process including knock, and they did not report on the details of the turbocharging aspect.

Turbocharger: Figure 2 is a schematic of the new system which includes the base engine, a compressor, an intercooler, and a turbine. The turbocharger is based on a wastegate and does not use a variable geometry turbine (VGT). The work of the turbine is exactly equal to the required work of the compressor. For most conditions, only a portion of the exhaust is needed for the turbine work. The excess exhaust flow is “by-passed” directly to the system discharge piping. New sources of exergy destruction (outside of the original engine system) are due to the compressor and turbine irreversibilities, and to flow past the exhaust valve. The irreversibilities of the flow past the intake valve are included with the original engine system and are already considered. In addition to these new irreversibilities, some exergy is removed with the energy transfer in the intercooler.

Without turbocharging and using the original control system, fuel vaporization was assumed to occur outside

of the engine cylinder contents. With turbocharging, the fuel is assumed to completely vaporize in the intake ports. The major effect of this feature is a temperature decrease of the incoming air-fuel vapor charge. For the conditions examined, this temperature decrease is of the order 20 K.

Engine: The engine selected for this study is an automotive, turbocharged, 3.8 liter, V-6 engine with a bore and stroke of 96.5 and 86.4 mm, respectively. This engine was selected as representative of this type of application, and some limited information was available on the engine specifications. Table 1 lists the engine specifications and table 2 lists some of the engine operating conditions and fuel parameters for the base case (2000 rpm, WOT). Some parameters were selected for simplicity and for comparison to previous studies of naturally aspirated engines, and may not be an exact match for any specific manufacturer. For example, the equivalence ratio was assumed to be stoichiometric ($\phi = 1.0$), and the combustion burn duration was assumed to be 60°CA. Start of combustion was determined for maximum brake torque (MBT). The use of these types of consistent conditions provided a less ambiguous comparison as other parameters were varied.

Again, for consistency and ease of comparison, for the base case, compressor and turbine isentropic efficiencies were assumed equal and constant at 65%. The intercooler effectiveness was assumed to be 60%. These values will be varied during parametric studies, but otherwise they are constant. Although not exactly true in applications, for purposes of this study these assumptions were useful. Table 3 is a list of the operating conditions as functions of engine speed for the wide open throttle (WOT) or full load conditions.

Results: This study examined the use of turbocharging for a spark ignition engine from both the first law and second law perspectives. Results are presented for detail and overall effects of turbocharging as functions of engine speed and load.

Table 1. Engine Specifications: Turbo

Item	Value
Number of cylinders	6
Bore (mm)	96.5
Stroke (mm)	86.4
Crank Rad/Con Rod	0.285
Compression Ratio	8.0:1
Inlet Valves:	
Diameter (mm)	41.3
Max Lift (mm)	8.75
Opens (°CA aTDC)	344
Closes (°CA aTDC)	-124
Exhaust Valves:	
Diameter (mm)	36.2
Max Lift (mm)	8.75
Opens (°CA aTDC)	110
Closes (°CA aTDC)	396
Valve Overlap (degrees)	52°

**Table 2. Engine and Fuel Input Parameters
For the Base Case: 2000 rpm, WOT, “MBT” timing**

Item	Value Used	How Obtained
Engine Speed (rpm)	2000	Input
Displaced Volume (dm ³)	3.791	Computed
AF _{stoich}	15.13	For isooctane
Fuel LHV (kJ/kg)	44,400	For isooctane
Equivalence Ratio	1.0	Input
Mechanical Frictional mep (kPa)	88.3	Algorithm
Inlet Pressure (kPa)	137.0	Input
Engine Exit Pressure – Turbine Inlet Pressure (kPa)	148.8	Input
Turbine Exit Pressure – Exhaust System Pressure (kPa)	105.0	Input
Start of Combustion (°bTDC)	24.5	For MBT
Combustion Duration (°CA)	60	Input
Cylinder Wall Temp (K)	450	Input
Compressor Inlet (ambient) Temperature and Pressure	310.3 K 100 kPa	Input
Compressor Isentropic Efficiency	65.0%	Input
Turbine Isentropic Efficiency	65.0%	Input
Intercooler Effectiveness	60.0%	Input
Coolant Inlet Temperature to Intercooler (K)	310.0	Input

Table 3. Operational Parameters for WOT

Speed (rpm)	ϕ	θ_b (°CA)	θ_o (°CA bTDC) (MBT)	p_{in} (kPa)	p_{exh} manifold (kPa)
1000	1.0	60	20.0	100.0	111.1
1200	1.0	60	20.0	105.2	115.3
1500	1.0	60	21.0	114.7	124.5
2000	1.0	60	24.0	137.0	148.8
2500	1.0	60	24.0	167.7	179.6
3000	1.0	60	24.5	167.7	205.0
3500	1.0	60	25.0	167.7	219.4
4000	1.0	60	25.5	167.7	226.0
4400	1.0	60	25.5	167.7	228.3

Figure 3. Inlet and exhaust manifold pressures as functions of engine speed for the WOT conditions.

Study Constraints: The following results are based on the assumptions and approximations described above. In addition, combustion stability, cycle-to-cycle variations, and other combustion issues are not included. Furthermore, knock, preignition, and other abnormal combustion

phenomena are not considered. As noted for each case, most parameters (such as MBT timing, equivalence ratio, ...) remain constant while one parameter is varied.

Figure 4. Inlet and exhaust manifold pressures as functions of engine load for 2000 rpm.

Prescribed Inlet and Exhaust Pressures: Figure 3 shows the prescribed inlet and exhaust manifold pressures as functions of engine speed for WOT conditions. The turbocharger is activated at 1000 rpm and the inlet manifold pressure increases up to 167.7 kPa at 2500 rpm. For higher engine speeds, the manifold pressure remains at 167.7 kPa. The exhaust manifold pressure continues to increase from about 100 kPa at low speeds to about 228.3 kPa at 4400 rpm due largely to the increases in the mass flow. Figure 4 shows the inlet and exhaust manifold pressures as functions of engine load for 2000 rpm.

Results for the Base Case Condition: As mentioned above, the base case operating conditions for this investigation included an engine speed of 2000 rpm, full load, MBT timing and an equivalence ratio of 1.0. Figure 5 shows the gas temperatures from the compressor inlet to the engine cylinder inlet. From the compressor inlet to the outlet, the gas temperature increases from 310.3 K to

351 K. The gases then flow through the intercooler and are cooled back down to 326 K. Finally, fuel is injected into the engine port and, due to the fuel vaporization, the gases are cooled down to 308 K.

In a similar fashion, figure 6 shows the gas temperatures from the engine exhaust port, through the turbine, through the by-pass (associated with the wastegate), and finally into the exhaust system. The gases leaving the engine for this condition have a temperature of 1134 K. About 61.5% (by mass) of the exhaust enters the turbine and the remaining gases by-pass the turbine. The gases exit the turbine with a temperature of 1079 K. The turbine exit gases are combined with the wastegate gases (1100 K), and the mixture enters the exhaust system.

Figure 7 shows the brake thermal efficiency as functions of the turbine and compressor isentropic efficiencies for three values of the intercooler effectiveness for the base case conditions. For simplicity, the turbine and compressor isentropic efficiencies were considered equal. As the component efficiencies increase or the intercooler effectiveness increases, the brake thermal efficiency increases slightly. One of the reasons for the increase of efficiencies with higher intercooler effectiveness is the resulting lower inlet temperatures.

Results as Functions of Speed and Load: Figure 8 shows the brake mean effective pressure (bmep) and the brake specific fuel consumption (bsfc) as functions of engine speed for the full load conditions. The bmep increases as speed increases up to 2500 rpm, then decreases slightly and then remains relatively constant for further increases of engine speed. The bsfc decreases as engine speed increases up to 2500 rpm, and then increases. These results reflect the net effects of decreasing relative heat transfer, increasing friction, and the inlet and exhaust pressure schedules as engine speed increases.

Figure 9 shows the brake mean effective pressure (bmep) and the brake specific fuel consumption (bsfc) as functions of engine load for 2000 rpm. As expected, the bmep increases linearly with load. The bsfc decreases with increases of engine load – the most decrease is due to the reduction of throttling for the part load conditions. Once the turbocharger is active, the decreases of bsfc are much less.

Figure 5. Gas temperatures from compressor inlet through to engine inlet.

Figure 7. Brake thermal efficiency as functions of component efficiencies for three values of the intercooler effectiveness for the base case conditions.

Figure 6. Gas temperatures from engine out through the turbine and into the exhaust system.

Figure 8. Brake mean effective pressure (BMEP) and brake specific fuel consumption (BSFC) as functions of engine speed for the WOT conditions.

Figure 9. Brake mean effective pressure (bmep) and brake specific fuel consumption (bsfc) as functions of load for the 2000 rpm case.

Figure 11. Brake thermal efficiency as a function of load (bmep) at 2000 rpm for three engine configurations.

Figure 10. Brake thermal efficiency as a function of brake power at 2000 rpm for three engine configurations.

Figure 10 shows the brake thermal efficiency as functions of the brake power for three engine configurations for the base case conditions. The turbocharged 3.8 liter engine is compared to a naturally aspirated (NA) 3.8 liter engine, and to a naturally aspirated 5.7 liter, V-8 engine. The latter engine has been extensively examined in a number of previous studies (e.g., [10–12]). The 5.7 liter engine has roughly the same design power as the turbocharged 3.8 liter engine. For a given brake power level, the 3.8 liter engine is more efficient due to the lower losses. Of particular significance, the 3.8 liter engine will have a more open throttle to achieve the same brake power thus reducing the pumping loss component of the losses. No effort was completed to try to optimize any of the engines other than by selecting the MBT spark timing. Other operating and design conditions may result in slightly different results.

Further, the maximum power of the 3.8 liter engine may be extended to nearly the maximum power of the 5.7 liter engine by the use of turbocharging while retaining some efficiency gains. Figure 10 captures the idea of “downsizing” discussed in the introduction.

On the other hand, figure 11 shows the brake thermal efficiency as a function of bmep for the three engine configurations. For a given bmep level, the efficiencies are roughly the same for all three engine configurations on this basis. This similarity of efficiencies is partly due to the consistent operating and design conditions selected. Further, the maximum bmep for each engine configuration reflects the specific designs. For example, the turbocharged 3.8 liter engine has the highest maximum bmep, and the naturally aspirated 3.8 liter engine has the lowest maximum bmep.

Second Law Results: Results were obtained for the base case (2000 rpm) based on both the first law and second law of thermodynamics. Table 4 lists the percentage of the fuel energy and fuel exergy associated with the various items. The fuel energy is divided between indicated work, engine heat transfer, exhaust gas, intercooler heat transfer, and unused fuel. The work associated with the compressor and turbine are not listed since for the complete system these are in balance.

Also listed in table 4 is the percentage of fuel exergy associated with the various items. The exergy percentage associated with the heat transfer (16.9%) is slightly less than the energy percentage (21.4%) since not all the heat transfer energy can produce work. Similarly, the exergy percentage associated with the exhaust flow (23.0%) is less than the energy percentage (40.9%). The major new items are the exergy destruction terms due to the turbocharger components. These terms include exergy destruction due to the compressor, turbine, and exhaust flow. As for the naturally aspirated case, exergy destruction due to combustion and the inlet flow remain.

The most significant of all the exergy destruction terms remains the combustion process. For these conditions, the destruction due to combustion is about 20.6% of the fuel exergy. The other destruction terms are much smaller. In order of decreasing importance, these are: exhaust valve flow (1.93%), inlet flow (1.44%), compressor (0.46%) and turbine (0.24%). In other words, the use of turbocharging does not significantly add to the overall irreversibilities.

**Table 4. Example Results for the Base Case:
2000 rpm, WOT, "MBT" timing**

Item	Energy (%)	Exergy (%)
Indicated Work	36.32	34.66
Heat Transfer	21.4	16.90
Net Flow Out	40.90	22.95
Intercooler Heat Transfer	0.95	0.11
Destruction Combustion	n/a	20.63
Destruction Compressor	n/a	0.46
Destruction Turbine	n/a	0.24
Destruction Inlet	n/a	1.44
Destruction Exhaust	n/a	1.93
Unused Fuel	0.68	0.67
	—	—
Total	100.0	100.0

Since the combustion irreversibilities are dominant, these have been examined in more detail. Figures 12 and 13 show the exergy destroyed by combustion as functions of engine load (at 2000 rpm) and speed (full load), respectively. As load and speed increases, the exergy destruction decreases – although the change is relatively modest. The range is rather small: between about 20.2% and 21.0%. These decreases are largely due to operating conditions which result in higher gas temperatures during combustion, and hence, less exergy destruction. These results are consistent with previous results for naturally aspirated engines – exergy destroyed by combustion decreases as the combustion temperatures increase which is the case for both increasing load and increasing speed.

A number of the features of the turbocharged system were evaluated from the perspective of the second law of thermodynamics. The following results are largely focused on the turbocharger features – previous literature [10–12] has provided results on the essential engine components.

Examples of the second law evaluations of the turbocharger components include the exergy destruction due to the compressor and turbine. Figure 14 shows the exergy destruction due to the compressor and turbine as functions of isentropic efficiency for the base case condition. In general, as the component efficiency increases, the exergy destruction decreases. For these conditions, the

exergy destruction is low, but the trends are of interest. The exergy destruction due to the turbine is lower than for the compressor since not all of the mass flows through the turbine.

Figure 15 shows the exergy destruction due to the compressor and turbine as functions of engine speed for the WOT conditions. The exergy destruction as a percentage of the fuel exergy increases with increases in speed for both components, but for the higher speeds the increase is much less. Again, the exergy destruction due to the turbine is less than for the compressor due to the lower flow rate through the turbine.

Another example of the results is presented in figure 16 which shows the flow exergy from the cylinder past the exhaust valve into the port, the flow exergy entering the port, and the exhaust mass flow rate as functions of crank angle for the base case. The exergy destruction due to flow past the exhaust valve is the difference between the cylinder flow exergy and the port flow exergy. This exergy destruction is largely due to the pressure loss and is proportional to the instantaneous mass flow rate. The exergy destruction is largely during the “blow down” portion of the exhaust event. The integrated value of the exergy destroyed due to the flow past the exhaust valve is listed in table 4 and accounts for 1.9% of the input fuel exergy for these conditions.

Figure 12. Exergy destroyed by combustion as a function of load for 2000 rpm.

Figure 13. Exergy destroyed by combustion as a function of engine speed for full load.

Figure 14. Exergy destruction due to the compressor and turbine as functions of the isentropic component efficiencies for the base case condition at 2000 rpm.

Figure 15. Exergy destruction due to the compressor and turbine as functions of the engine speed.

Figure 16. Flow exergy and exhaust flow rate as functions of crank angle for the base case.

Figure 17. Exhaust energy (at exhaust port exit) as a function of load (bmeP) at 2000 rpm for three engine configurations.

Figure 18. Exhaust exergy (at exhaust port exit) as a function of load (bmep) at 2000 rpm for three engine configurations.

For completeness, figures 17 and 18 show the exhaust energy and exergy (at the port exit) for the three engines described above. The 5.7 liter, naturally aspirated engine has the highest energy and exergy values. This is due to the higher flow rates. The two versions of the 3.8 liter engine have exhaust values which overlap as expected. In general, both sets of results (figures 17 and 18) illustrate the potential for exhaust energy/exergy recovery.

Figure 19 shows the percentage of the fuel energy which is in the exhaust gases at the port exit and at the turbine exit as a function of load (bmep) for an engine speed of 2000 rpm and an equivalence ratio of 1.0 with MBT spark timing. At the port exit, the exhaust energy as a percentage of the fuel energy increases as load increases. This is mostly due to the lower percentage heat losses as load increases, and some of this energy is retained in the cylinder gases – thus increasing the exhaust gas energy. For the range of loads where the turbocharger is active, the energy of the exhaust gases at the turbine exit are lower than at the port. The difference represents the energy extracted by the turbine to provide shaft work to drive the compressor for these conditions.

At the WOT condition, slightly more than 1.5% of the fuel energy is extracted by the turbine.

Figure 19. Exhaust energy at exhaust port exit and turbine exit as functions of load (bmep) at 2000 rpm.

Figure 20. Percentage of the fuel exergy represented by the exhaust streams as functions of load (bmep) at 2000 rpm.

Figure 22. Percentage of the fuel exergy represented by the exhaust streams as functions of engine speed for full load.

Figure 21. Exhaust energy at exhaust port exit and turbine exit as functions of engine speed for full load.

Figure 20 shows the percentage of the fuel exergy which is in the exhaust gases at the port exit and at the turbine exit as a function of load (bmep) for the same conditions as for figure 1. The exergy values are significantly lower than the energy values since not all of the energy is available to do work. Further, the amount of exergy extracted by the turbine for the same conditions is greater – about 2% of the fuel exergy at the WOT condition. This greater percentage is because some of the exergy is lost due to the destruction of exergy by the turbine. The remaining exergy delivered by the turbine is equal to the turbine work. The exergy destroyed as a percentage of the fuel exergy is represented in the figure by the hatched space below the port exit exhaust exergy line.

Figures 21 and 22 are similar to figures 19 and 20 except these figures show the energy and exergy, respectively, at the port exit and at the turbine exit as functions of engine speed for full load. For the full load conditions, the turbocharger is active for speeds greater than 1000 rpm. Again, the difference between the two curves represents the work delivered by the turbine to drive the

compressor for these conditions. Figure 22 shows the exergy at the port exit, the exergy at the turbine exit, and the exergy destroyed in turbine.

Conclusions: This investigation has presented results from both a first law and a second law perspective for a turbocharged, spark-ignition engine. A major objective of the current work was to better understand the trade-offs and the fundamental aspects of a turbocharged engine. This was accomplished by determining the energy and exergy quantities for a range of operating conditions for a spark-ignition engine. A 3.8 liter automotive engine with a turbocharger and intercooler was selected for this study.

- For the base case (2000 rpm and a bmep of 1200 kPa), the bsfc was about 240 g/kW-h (33.8% brake thermal efficiency).
- At the base case conditions, the second law analysis indicated that the original fuel exergy was distributed as follows: 34.7% was indicated work,

16.9% was moved via heat transfer to the cylinder walls, 23.0% exited with the exhaust gases, 20.6% was destroyed during the combustion process, 2.5 % was destroyed due to inlet mixing processes, and 1.9% was destroyed due to the exhaust processes.

- The turbocharger components including the inter-cooler were responsible for less than 1.0% of the fuel exergy destruction or transfer.
- A comparison of three engines with and without turbocharging quantified the advantages of “downsizing.” That is, the use of a smaller, turbocharged engine can provide efficiency advantages relative to a larger, non-turbocharged engine for the same power level. When compared on a bmep basis, however, the three engines had similar efficiencies.
- Although the magnitudes were small, increasing the isentropic efficiencies of the compressor and turbine decreased the exergy destruction.

Appendix A:

Publications from 2005 through Present (reverse chronological)

1. J. A. Caton, "A Thermodynamic Evaluation of the Use of Alcohol Fuels in a Spark-Ignition Engine," accepted for publication and presentation at the 2009 SAE Powertrains, Fuels and Lubricants Meeting, Society of Automotive Engineers, SAE paper no. 2009-01-2621, Grand Hyatt San Antonio, San Antonio, TX, 02-04 November 2009
2. J. A. Caton, "The Use of an Engine Cycle Simulation to Examine Alcohol Fuels for a Spark-Ignition Engine," in the Proceedings of the 2009 Spring Technical Conference, Central States Section of the Combustion Institute, 6th U. S. National Combustion Meeting, Ann Arbor, MI, 17-20 May 2009.
3. J. A. Caton, "A Turbocharged, Spark-Ignition Engine: Results from an Engine Cycle Simulation Including the Second Law of Thermodynamics," Proceedings of the 2009 Spring Technical Conference of the ASME Internal Combustion Division, paper no. ICES2009-76023, InterContinental Milwaukee Hotel, Milwaukee, WI, 03-06 May 2009.
4. R. G. Shyani, and J. A. Caton, "Results from a Thermodynamic Cycle Simulation for a Range of Inlet Oxygen Concentrations Using Either EGR or Oxygen Enriched Air for a Spark-Ignition Engine," 2009 SAE International Congress and Exposition, Society of Automotive Engineers, Cobo Hall, Detroit, MI, SAE paper no. 2009-01-1108, 20-23 April 2009.
5. R. G. Shyani, and J. A. Caton, "A Thermodynamic Analysis of the Use of EGR in SI Engines Including the Second Law of Thermodynamics," *Proceedings of the Institution of Mechanical Engineers, Part D, Journal of Automobile Engineering*, vol. 223, no. 1, pp. 131-149, 2009.
6. J. A. Caton, "Results from an Engine Cycle Simulation of Compression Ratio and Expansion Ratio Effects on Engine Performance," *ASME Transactions — Journal of Engineering for Gas Turbines and Power*, Vol. 130, pp. 052809-1 to 052809-7, September 2008.
7. H. Sivadas and J. A. Caton, "Effects of Exhaust Gas Recirculation on Exergy Destruction due to Isobaric Combustion for a Range of Conditions and Fuels," *International Journal of Energy Research*, vol. 32, pp. 896-910, 2008.
8. K. T. Patrawala and J. A. Caton, "Potential Processes for "Reversible" Combustion with Application to Reciprocating Internal Combustion Engines," in proceedings of the 2008 Spring Technical Conference of the Central States Section of the Combustion Institute, Tuscaloosa, AL, 20 - 22 April 2008.
9. R. G. Shyani, T. J. Jacobs, and J. A. Caton, "On the Quantitative Deficiencies of Ideal Air-Standard Engine Cycles," in proceedings of the 2008 Spring Technical Conference of the Central States Section of the Combustion Institute, Tuscaloosa, AL, 20 - 22 April 2008.
10. J. A. Caton, "The Effects of Compression Ratio and Expansion Ratio on Engine Performance Including the Second Law of Thermodynamics: Results from a Cycle Simulation," in *Proceedings of the 2007 Fall Conference of the ASME Internal Combustion Engine Division*, Charleston, SC, 14-17 October 2007.
11. P. S. Chavannavar, and J. A. Caton, "The Destruction of Availability (Exergy) due to Combustion Processes: A Parametric Study," *Journal of Power and Energy, Proceedings of the Institution of Mechanical Engineers, Part A*, vol. 220, number 7, pp. 655-669, 2006.
12. J. A. Caton, "Utilizing a Cycle Simulation to Examine the Use of EGR for a Spark-Ignition Engine Including the Second Law of Thermodynamics," in *Proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division*, Sacramento, CA, 5-8 November 2006.
13. J. A. Caton, "First and Second Law Analyses of a Spark-Ignition Engine Using Either Isooctane or Hydrogen," in *Proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division*, Sacramento, CA, 5-8 November 2006.

14. J. A. Caton, "The Effects of Exhaust Gas Recirculation (EGR) for a Spark-Ignition Engine: A Second Law Analysis," in *Proceedings of the 2006 Spring Meeting of the Central States Section of the Combustion Institute*, Cleveland, OH, 21–23 May 2006.
15. P. S. Chavannavar and J. A. Caton, "Irreversibilities Associated with Basic Combustion Processes," in *Proceedings of the 2006 Spring Meeting of the Central States Section of the Combustion Institute*, Cleveland, OH, 21–23 May 2006.

Theses and Dissertations

1. Vaibhav J. Lawand, "Use of a Thermodynamic Engine Cycle Simulation to Study a Turbocharged Spark-Ignition Engine," MSME, December 2009.
2. Rajeshkumar Shyani, "An Investigation of the Use of EGR for Spark-Ignition Engines: Using an Engine Cycle Simulation," MSME, August 2008.
3. Sushil Oak, "Use of an Engine Cycle Simulation to Study Diesel Engine Combustion," MSME, August 2008.
4. Hari Sivadas, "The Effects of EGR, Water/N₂/CO₂ Injection, and Oxygen Enrichment on the Availability Destroyed Due to Combustion for a Range of Conditions and Fuels," MSME, August 2007.
5. Kaushik T. Patrawala, "An Examination of Possible Reversible Combustion at High Temperatures and Pressures for a Reciprocating Engine," MSME, May 2007.
6. Dushyant Pathak, "Use of a Thermodynamic Cycle Simulation to Determine the Difference Between a Propane-Fuelled Engine and an Iso-Octane-Fuelled Engine," MSME, December 2005.

Appendix B:

Example Publication Concerning the Simple Systems

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Destruction of availability (exergy) due to combustion processes: a parametric study

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Abstract: An analytical examination of the destruction of availability was completed for constant pressure, constant volume, and constant temperature combustion processes for iso-octane vapour and air mixtures. The variation of the percentage destruction of availability was determined as a function of temperature, pressure, and equivalence ratio. The percentage destruction of availability decreased with increasing reactant temperatures (from ~30 per cent at 300 K to ~5 per cent at 4500 K for constant pressure and constant volume combustion processes). The effect of the reactant pressure on the percentage availability destroyed was less pronounced – for example, for a 500 K initial temperature, a change from 50 to 5000 kPa changed the percentage availability destroyed from 26 per cent to 22 per cent for constant pressure adiabatic combustion. For changes in the equivalence ratio, the lowest destruction of availability was for mixtures near stoichiometric. In addition, the contribution of the various components (e.g. chemical and thermo-mechanical) of the mixture availability to the total availability was quantified for a range of conditions. Also, the effect of the decomposition of the reactant species for high reactant temperatures (greater than 3000 K) was determined.

Keywords: combustion, destruction of exergy, chemical availability, fuels

1 INTRODUCTION

Modern society is heavily dependent on fossil fuels as a source of energy. The energy present in these fossil fuels arises from the chemical energy of the molecules. Combustion is the most popular process used to liberate this chemical energy present in the fuels. Combustion, however, is an irreversible process with corresponding losses of availability[†] (or exergy) associated with the process [1–8]. Some work has been done on studying the loss of availability during combustion by Dunbar and Lior (for constant pressure combustion processes) [4], by Caton (constant volume combustion processes) [5], and Daw *et al.* (constant pressure combustion

processes) [6]. These and other previous studies are summarized below.

Second-law analyses of combustion processes are particularly valuable, as they aid in understanding the various causes of irreversibility during the processes and in determining the maximum theoretical efficiency of the process. The aim of this paper is to examine the various parameters affecting the destruction of availability during different, relatively simple combustion processes (constant pressure, constant volume, and constant temperature). The current work expands and extends previous work [4–6], and provides a self-consistent format for comparisons of a number of processes. One of the major motivations for this study is that it would lead to the identification and subsequent implementation of combustion strategies to reduce availability losses during the various combustion processes.

The next subsection will discuss the concept of availability, chemical availability, and related previous work. This will be followed by sections on the

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[†]Availability (exergy) is described in detail in a subsequent section.

analytical approach, results and discussion, and summary and conclusions.

1.1 Availability

Availability is a measure of the energy in a system that is available for useful work. This thermodynamic property is also referred to as exergy by a number of authors [1–4]. Availability is a better measure of the work potential of a system compared to properties such as internal energy or enthalpy of the system. No device or process can extract a quantity of work greater than the availability of the system without violating the second law of thermodynamics. Availability may be divided into three types – thermal, mechanical, and chemical – each representing the potential for work as the system comes to thermal, mechanical, and chemical equilibrium with the environment, respectively. The availability of a system, therefore, is dependent on the chosen environment. For purposes of determining the availability values, the parameters of the environment must be precisely defined. Once a thermodynamic system is in equilibrium with the environment, no further work can be obtained. This is why the state of the environment is also called the dead state [1–3].

The process of determining the availability of a system may be considered a two-step procedure: (a) that of determining the thermo-mechanical availability and (b) that of determining the chemical availability of the system.

The thermo-mechanical availability is evaluated with respect to a 'restricted dead state.' The restricted dead state is achieved by allowing the system to come to thermal and mechanical equilibrium with the environment, typically the surrounding atmosphere. The restricted dead state, therefore, has the same temperature and pressure as the environment. The composition of the restricted dead state, however, corresponds to the original system composition and is not necessarily the same as that of the environment (dead state).

Following usual conventions [1–8], the thermo-mechanical availability of a system is defined as

$$A_{TM} = (U - U^0) - T_0(S - S^0) + P_0(V - V^0) \quad (1)$$

where A_{TM} , U , S , and V are the thermo-mechanical availability, internal energy, entropy, and volume of the system, respectively, and the superscripts 0 denote corresponding properties of the restricted dead state. T_0 and P_0 are the temperature and pressure of the environment, respectively.

The chemical availability of a system is the work potential present due to any differences in the composition (and concentration of the species) of the

system and the environment. Once again, following usual conventions [1–8], the chemical availability may be defined as

$$A_{Ch} = \sum_{k=1}^n N_k(\mu_k^0 - \mu_{k,0}) \quad (2)$$

where A_{Ch} is the chemical availability of the system. N_k is the number of moles of component k in the system. μ_k^0 and $\mu_{k,0}$ are the chemical potentials of component k in the restricted dead state and the environment, respectively.

The chemical potential of the various species in the restricted dead state may further be expressed as

$$\mu_k^0 = g_k(T_0, P_0) + \bar{R}T_0 \ln\left(\frac{p_k^0}{p_{k,0}}\right) \quad (3)$$

where $g_k(T_0, P_0)$ is the Gibbs energy of pure component k , $\bar{R}$ the universal gas constant, p_k^0 and $p_{k,0}$ the partial pressures of component k in the restricted dead state and the atmosphere, respectively. Consideration of the mixed species is included in the 'ln' term.

The chemical availability term can further be split into two components, designated here as 'reactive availability' and 'diffusion availability'. Reactive availability is the availability due to the difference in composition of the restricted dead state and the atmosphere, whereas diffusion availability is the availability due to the difference in concentrations of the species in the restricted dead state and the atmosphere. In other words, the reactive availability accounts for the work that could be produced as the species (such as carbon monoxide) react to form species consistent with the environment (such as carbon dioxide). The expressions for these two components would then be

$$A_{Re} = \sum_{i=1}^{n^0} N_i g_i(T_0, P_0) - \sum_{j=1}^{n_0} N_j g_j(T_0, P_0) \quad (4)$$

$$A_{Diff} = \bar{R}T_0 \sum_{j=1}^n N_j \ln\left(\frac{p_j^0}{p_{j,0}}\right) \quad (5)$$

where the index i represents the individual constituents in the restricted dead state and the index j represents the individual species in the mixture, obtained after converting the species present in the restricted dead state into species present in the environment (dead state). To complete a determination of the chemical availability, the concentration of the species in the environment (dead state) must be known.

Thus, in summary

$$A_{\text{Total}} = A_{\text{TM}} + A_{\text{Re}} + A_{\text{Diff}} \quad (6)$$

Also note that for open systems, the flow availability is used, and is defined as

$$A_{\text{TM},f} = (H - H^0) - T_0(S - S^0) \quad (7)$$

where H and H^0 are the enthalpies of the system and the restricted dead state, respectively.

1.2 Previous work

Although a large amount of work has been done on availability analysis of engines [9], turbines, and power plants [2], relatively little work has been done towards studying the ideal combustion processes themselves. Dunbar and Lior [4] examined the case of constant pressure adiabatic combustion. In particular, Dunbar and Lior [4] examined the various contributions to the destruction of availability by dividing the combustion process into a number of hypothetical subprocesses. The hypothetical subprocesses considered in the analysis were (a) combined diffusion/fuel oxidation, (b) 'internal thermal energy exchange' (heat transfer), and (c) the product constituent mixing process. The largest contributor to the destruction of availability was found to be due to the internal energy exchange within the system. The fuels considered by Dunbar and Lior [4] during their analysis were hydrogen and methane.

Caton [5] conducted an analysis of constant volume combustion, with particular emphasis on the implications of the results as applicable to internal combustion engines. Caton [5] analysed the combustion of iso-octane for a range of reactant temperatures, pressures, and equivalence ratios. In general, the destruction of availability decreased with increasing reactant temperatures and increasing equivalence ratios. The effect of reactant pressure on the destruction of availability was relatively modest, when compared with the other parameters.

Daw *et al.* [6] examined a conceptual isobaric combustion process with reduced combustion irreversibility. Their work primarily focused on the effect of preheating the reactants on reducing the irreversibility losses during the combustion process. The high temperature exhaust gases were used in a counter flow heat exchanger to heat the reactant fuel-air stream, thus reducing the destruction of availability due to the internal thermal energy exchange during the combustion process.

Richter and Knoche [7] also examined the possibility of reversible combustion, using metal oxides

as intermediaries. Their work also compared the availability losses for constant pressure, constant volume, and constant temperature combustion. This is useful in identifying which combustion process is more effective in terms of the destruction of availability due to combustion. Richter and Knoche [7] concluded that for reactants starting at room temperature and atmospheric pressure, the exergy losses were greatest for a constant pressure combustion process and least for constant temperature isothermal combustion.

One aspect found lacking in most of the previous studies is the formal evaluation of the chemical availability of the system. An example of the formal use of the chemical availability component in an availability analysis was completed by Van Gerpen and Shapiro [8], who outlined the need for including the chemical availability component, as this term increases in significance with increasing temperatures and richer equivalence ratios due to increased concentrations of incomplete products of combustion, such as carbon monoxide and hydrogen, which are not present in the atmosphere. For rich mixtures, therefore, the reactive availability was significant for the cases they studied.

2 ANALYTICAL APPROACH

The current work examines constant pressure, constant volume, and constant temperature combustion. Figure 1 shows schematic diagrams for these combustion processes. During constant pressure and constant volume combustion, the reactants and products are maintained at the same pressure and volume, respectively, with no work or heat transfer across the system boundary. During constant temperature combustion, the reactants and products are maintained at the same temperature; however, this necessitates some heat transfer, Q , across the system boundary, while the work done is still zero.

2.1 Assumptions and approximations

The following assumptions and approximations were used during the course of this work:

- adiabatic combustion conditions were assumed during constant pressure and constant volume combustion processes;
- the products of combustion had enough time to attain the equilibrium mixture composition;
- ideal gas behaviour;
- distributions of the various species and the pressure and temperature in the combustion chamber were uniform;

Fig. 1 Schematic of various combustion processes

- (e) species considered for the equilibrium product mixture consisted of CO_2 , CO , H_2O , OH , H_2 , H , O_2 , O , N_2 , N , NO , NO_2 , and Ar .

2.2 Thermodynamic properties

The thermodynamic properties for the various computations were obtained using polynomial curve fits to the thermodynamic data [10]. The mixture composition itself was determined from equilibrium considerations. The algorithm used for determination of these equilibrium compositions is described in detail elsewhere [11].

The reactant and product mixture properties (enthalpy, internal energy, and entropy) were then calculated from the following relations

$$H = \sum_{k=1}^n n_k h_k \quad (8)$$

$$U = \sum_{k=1}^n n_k u_k \quad (9)$$

$$S = \sum_{k=1}^n n_k \left[s_k(T) - \bar{R} \ln \left(\frac{p_k}{p_0} \right) \right] \quad (10)$$

where h_k , u_k , and s_k are enthalpy, internal energy, and entropy of component k , respectively.

2.3 Ambient conditions

As mentioned previously, determination of the availability requires the definition of the ambient conditions (dead state). For the purposes of this study, a standard 'wet' atmosphere was considered as the ambient condition. Table 1 gives the composition of this atmosphere. The atmospheric pressure and temperature were set as 101.325 kPa and 298.15 K, respectively.

The pressure and temperature of the restricted dead state is, therefore, 101.325 kPa and 298.15 K. The composition of the restricted dead state is the same as that of the system.

2.4 Destruction of availability

The change in availability of the mixtures was computed using an availability balance. The fraction of availability destroyed during combustion was given by the difference in the total reactant availability and the total product availability. For constant temperature combustion, some availability, A_T , is associated with the heat transfer, Q , across the system boundary. This was computed as

$$A_T = Q \left(1 - \frac{T_0}{T} \right) \quad (11)$$

where the term $(1 - T_0/T)$ is essentially the Carnot efficiency.

Performing an availability analysis on the system, the destruction of availability due to combustion, A_{Dest} , may be determined as follows

$$A_{\text{Dest}} = A_{\text{Initial}} - A_{\text{Final}} - A_T - A_W \quad (12)$$

where A_{Initial} and A_{Final} are the system availability before and after the combustion process, respectively. A_W is the availability associated with the work done during the combustion process. As no work interaction is allowed to occur for the combustion processes examined in this study, the term A_W is always zero. The term A_T is non-zero only for constant temperature combustion processes. Considering only the thermo-mechanical availability of

Table 1 Standard wet atmospheric composition used in the analyses

Species	Percentage (mole fractions)
Nitrogen, N_2	0.7565
Oxygen, O_2	0.2029
Carbon dioxide, CO_2	0.0003
Water, H_2O	0.0313
Argon, Ar	0.0090

the system

$$\begin{aligned} A_{\text{Initial, TM}} &= H_R - T_0 S_R \\ &\text{for isobaric combustion processes} \\ &= U_R - T_0 S_R + P_0 V \\ &\text{for isochoric combustion processes} \end{aligned} \quad (13)$$

$$\begin{aligned} A_{\text{Final, TM}} &= H_P - T_0 S_P \\ &\text{for isobaric combustion processes} \\ &= U_P - T_0 S_P + P_0 V \\ &\text{for isochoric combustion processes} \end{aligned} \quad (14)$$

where H_R , H_P , U_R , and U_P denote the reactant and product enthalpy and internal energy, respectively; T_0 and P_0 are the dead state (atmosphere) temperature and pressure; and V is the volume of the system. Therefore

$$\begin{aligned} A_{\text{Dest, TM}} &= A_{\text{Initial, TM}} - A_{\text{Final, TM}} \\ &\text{for constant pressure and constant} \\ &\text{volume combustion processes} \end{aligned} \quad (15)$$

$$\begin{aligned} A_{\text{Dest, TM}} &= A_{\text{Initial, TM}} - A_{\text{Final, TM}} - A_T \\ &\text{for constant temperature} \\ &\text{combustion processes} \end{aligned} \quad (16)$$

Equations (15) and (16) may be simplified and expressed in terms of the basic thermodynamic properties.

$$\begin{aligned} A_{\text{Dest, TM}} &= T_0 \Delta S \\ &\text{for constant pressure and constant} \\ &\text{volume combustion processes} \end{aligned} \quad (17)$$

$$\begin{aligned} A_{\text{Dest, TM}} &= T_0 \Delta S - Q \left(1 - \frac{T_0}{T} \right) \\ &\text{for constant temperature} \\ &\text{combustion processes} \end{aligned} \quad (18)$$

Equations (17) and (18) also serve as an internal consistency check during the computation of the values of the thermo-mechanical component of the availability destroyed. The percentage availability destroyed, r_{DAC} , was calculated as

$$r_{\text{DAC}} = \left(\frac{A_R - A_P}{A_R} \right) \times 100 \quad (19)$$

The above expression is valid for constant pressure and constant volume combustion. For constant temperature combustion, the percentage availability

Table 2 Fuel properties

Fuel	Iso-octane (C_8H_{18})
Molecular weight (kg/kmol)	114.14
Lower heating value (kJ/kg)	44 652
Fuel availability (kJ/kg)	45 750
Stoichiometric mass air-fuel ratio	15.14

destroyed, r_{DAC} , was calculated as

$$r_{\text{DAC}} = \left(\frac{A_R - A_P - A_T}{A_R} \right) \times 100 \quad (20)$$

The values of A_R and A_P in equations (19) and (20) represent the total (thermo-mechanical and chemical) availability of the system and, therefore, the calculated value of r_{DAC} denotes the total percentage of availability destroyed due to combustion.

3 RESULTS AND DISCUSSION

For this study, mixtures of iso-octane vapour and air were considered. Iso-octane is a fairly typical hydrocarbon fuel and has been used in previous studies [5]. Table 2 lists the properties of iso-octane used in this study. Other fuels also have been studied, and these results are presented elsewhere [12].

First, examples of the specific availability for the reactants and products for iso-octane-air mixtures for a range of reactant temperatures and pressures for an equivalence ratio of 1.0 will be described. Figure 2 shows the specific availability of the reactant mixtures as functions of reactant temperature for four reactant pressures. The availability values

Fig. 2 Reactant mixture availability as functions of reactant temperature for four reactant pressures for an equivalence ratio of 1.0

increase with increasing temperatures, reflecting the increase in the thermo-mechanical availability of the mixtures. With increasing temperatures, the availability curves diverge—with the availability values decreasing with increasing pressure. This is due to the decrease in the values of the specific volume at higher pressures. An increase in the pressure also leads to a reduction in the mixture entropy (and therefore, an increase in the mixture availability). This decrease, however, is a logarithmic function of the pressure and, therefore, is overshadowed by the decrease in the value of the specific volume.

Figure 3 shows the specific availability of the product mixtures (at chemical equilibrium) for the same range of pressures as functions of product temperature. Although the trend displayed is similar to that of the reactant mixtures, the availability values show a more rapid increase past 2500 K. This is due to the formation of incomplete products of combustion (dissociation) at these elevated temperatures. For higher pressures, this dissociation is suppressed, resulting in decreasing availability values. In the following results, the temperature of the product mixture is a function of initial reactant conditions and the combustion process (constant volume or constant pressure or constant temperature).

3.1 Constant pressure combustion process

Figure 4 shows the percentage (flow) availability destroyed for constant pressure combustion as functions of the reactant temperature for three reactant pressures. The percentage availability destroyed decreases with increasing reactant temperatures from ~27 per cent for a reactant temperature of 300 K to ~5 per cent for a reactant temperature of

Fig. 3 Product mixture availability (at chemical equilibrium) as functions of product temperature for five product pressures for an equivalence ratio of 1.0

Fig. 4 Percentage availability destroyed as functions of reactant temperature for three reactant pressures for constant pressure combustion

4500 K. Also, the percentage availability destroyed decreases with increasing pressure, but this effect is much more modest. The effect of varying the pressure from 50 to 5000 kPa causes a variation of <5 per cent of the total reactant mixture availability on the values of percentage availability destroyed during combustion. The decreased destruction of availability at higher reactant temperatures is due to the reduction in irreversibility at these higher temperatures. In general, the higher the temperatures, the lower the irreversibility. In other words, higher temperatures preserve more of the original availability. This is consistent with the results from the analysis of constant pressure combustion processes by Dunbar and Lior [4]. Note that for these and the following results, the current analysis does not account for any destruction of availability due to the preheating of the reactant mixture.

Figure 5 shows the percentage availability destroyed due to combustion as functions of the reactant temperature for three equivalence ratios (0.1, 0.5, and 1.0) for a reactant pressure of 500 kPa. For a reactant mixture temperature of 300 K, the percentage availability destroyed was greatest for the equivalence ratio of 0.1 and was least for the equivalence ratio of 1.0. This is because the richer (but still lean) mixtures result in higher product mixture temperatures, thus destroying smaller fractions of the reactant mixture availability. This trend changes at higher reactant temperatures. For reactant temperatures >2500 K, this trend is completely reversed, with the least destruction of availability occurring due to combustion of reactant mixtures with equivalence ratio of 0.1, and the greatest fraction of availability being destroyed during combustion of reactant mixture with an equivalence ratio of 1.0.

Fig. 5 Percentage availability destroyed as functions of reactant temperature for three lean equivalence ratios for constant pressure combustion of iso-octane for a reactant pressure of 500 kPa

Fig. 6 Percentage availability destroyed as functions of reactant temperature for three rich equivalence ratios for constant pressure combustion of iso-octane for a reactant pressure of 500 kPa

The differences, however, are small for the highest temperatures. This reversal of the trend at higher temperatures is because as the temperature increases the contribution of the reactive availability (the major part of the chemical availability) to the total availability becomes less and less important. For the lean mixtures, therefore, the ratio of the destroyed availability and the initial availability is a smaller number. As a consequence, the fraction of availability destroyed due to combustion is lesser for the leaner reactant mixtures at higher temperatures.

This observation is consistent with the sharp decrease of the destroyed availability for an equivalence ratio of 0.1 for temperatures less than ~ 1000 K. This sharp decrease is indicative of the smaller amount of reactive availability for this lean mixture, and the irreversibilities are sufficient to destroy most of this availability at these lower temperatures. For higher temperatures (greater than ~ 2500 K), dissociation becomes important and reactive species in the product mixture are responsible for the decreasing rate of change of the destruction percentage.

Figure 6 shows the percentage of availability destroyed due to combustion as functions of reactant temperature for equivalence ratios of 1.0, 1.5, and 2.0 for a reactant pressure of 500 kPa. Corresponding to a reactant mixture temperature of 300 K, the percentage of availability destroyed is greatest for the reactant mixture with an equivalence ratio of 1.0 and least for the mixture with equivalence ratio of 2.0. With increasing temperatures, the values for the percentage availability destroyed for the various equivalence ratios converge.

The lower values for the percentage availability destroyed due to combustion for richer equivalence ratios does not imply that combustion of rich mixtures is to be preferred. The values for equivalence ratios greater than 1.0 include the reactive availability (chemical energy) present in the product mixture because of the presence of the incomplete products of combustion. To make use of this availability in practical applications, additional combustion processes would be required and may not always be feasible. If this availability, which results from the incomplete products of combustion, is neglected in the availability balance, it is found that the fraction of availability destroyed is least for a near stoichiometric reactant mixture (see Fig. 7 and related discussion).

Figure 7 shows the product mixture temperature and the percentage of the reactant mixture availability destroyed as functions of the reactant mixture equivalence ratio for a pressure of 500 kPa and a reactant mixture temperature of 300 K. The product mixture temperature increases initially with increasing equivalence ratios, before decreasing once again. The peak product mixture temperature was for an equivalence ratio of approximately 1.03. Figure 7 shows two lines for the percentage availability destroyed due to combustion – the dashed line (1) represents the values obtained using the availability procedure described previously in section 2.4, whereas the solid line (2) represents the values for the percentage availability destroyed obtained by neglecting the reactive availability of the product mixture (chemical energy of the incomplete products

Fig. 7 Percentage availability destroyed and product mixture temperature as functions of equivalence ratio for constant pressure combustion of iso-octane for a reactant pressure of 500 kPa and a reactant temperature of 300 K.

of combustion). The dashed line (1) shows that the percentage of availability destroyed decreases with increasing equivalence ratios. This is because of the reduced irreversibility associated with the combustion of the richer reactant mixtures. Again, the combustion of richer equivalence ratios ($\phi > 1$) destroys smaller fractions of the reactant availability, but may not be of practical significance, as the availability present in the product gases is in the form of chemical energy (associated with the incomplete products of combustion). To liberate this energy, further combustion processes would be needed. The solid line (2) shows the variation in the fraction of reactant availability destroyed due to combustion with the availability resulting from the incomplete products of combustion neglected. Combustion of the reactant mixture with an equivalence ratio of about 0.9 results in the least destruction of the reactant availability. Note that combustion of a stoichiometric mixture also leads to formation of some amount of incomplete products of combustion and, therefore, a stoichiometric mixture does not result in the minimum destruction of availability for these conditions.

3.2 Constant volume combustion process

Figure 8 shows the percentage availability destroyed due to combustion as functions of the reactant mixture temperatures for reactant pressures of 50, 500, and 5000 kPa. Again, the effect of reactant temperature on the percentage of availability destroyed is much more pronounced when compared with the effect of the reactant mixture pressure. The values

Fig. 8 Percentage availability destroyed as functions of reactant temperature for three reactant pressures for constant volume combustion

of percentage availability destroyed due to combustion drop from ~ 25 per cent at 300 K to ~ 6 per cent at 4500 K. The destruction of availability decreases with increasing temperatures because of reduced irreversibility at higher temperatures, as described previously. This is due to the reduced losses associated with the internal thermal energy exchange (heat transfer) in the mixtures during the combustion process. The effect of the reactant pressure on the availability destroyed for constant volume combustion is more complex, causing the curves for the different pressures to intersect. This is mostly because of the specific volume term in the reactant and product mixture availability expressions.

Figure 9 shows the percentage availability destroyed as a function of reactant temperature for equivalence ratios of 0.1, 0.5, and 1.0 for a reactant pressure of 500 kPa. For a reactant temperature of 300 K, the destruction of availability is least for the reactant mixture with an equivalence ratio of 1.0, and greatest for the reactant mixture with an equivalence ratio of 0.1. This trend changes with increasing temperatures, and at higher temperatures, past 3500 K, this trend is completely reversed. The reasoning is once again similar to that for the constant pressure combustion processes. At lower temperatures, the destruction of availability is greatest for equivalence ratio of 0.1, as the final product temperature is lower, leading to greater availability losses due to internal thermal energy exchange as described by Dunbar and Lior [4]. At higher temperatures (> 1000 K), the trend reverses, as the reactive availability component is less significant in the leaner reactant mixtures.

Figure 10 shows the percentage availability destroyed as a function of reactant temperature for

Fig. 9 Percentage availability destroyed as functions of reactant temperature for three lean equivalence ratios for constant volume combustion of iso-octane for a reactant mixture pressure of 500 kPa

equivalence ratios of 1.0, 1.5, and 2.0 for a reactant pressure of 500 kPa. At the lower reactant mixture temperatures, the destruction of availability is greatest for the mixture corresponding to an equivalence ratio of 1.0, with the values converging for higher reactant mixture temperatures >4000 K. Once again, the percentage availability destroyed is lower for the richer reactant mixtures as long as the reactive availability of the product mixture is included in the availability balance. If this availability is not

Fig. 10 Percentage availability destroyed as functions of reactant temperature for three rich equivalence ratios for constant volume combustion of iso-octane for a reactant pressure of 500 kPa

included, then the stoichiometric mixture once again leads to the least destruction of availability due to combustion. As with the constant pressure combustion process, combustion of rich mixtures is not necessarily desired, as the reactive availability can be significant in the products.

Figure 11 shows the variation in the percentage availability destroyed and the product mixture temperature as a function of the equivalence ratio. The product mixture temperatures increase with increasing equivalence ratios, before dropping once again with further increase in the equivalence ratios. The maximum product mixture temperature was found to occur corresponding to an equivalence ratio of approximately 1.1. This is because of the formation of the incomplete products of combustion, which require less than the stoichiometric amount of air for combustion. Figure 11 also shows two lines for the percentage availability destroyed due to the combustion process. The dashed line (1) shows the values for the percentage availability destroyed, computed as described in section 2.4. The values for the percentage availability destroyed decrease monotonically with increasing equivalence ratios. The solid curve (2) shows the values for the percentage availability destroyed, ignoring the reactive availability of the products. If the reactive availability component for the products is not included in the availability balance, the trend changes – with the least destruction of availability for combustion of the reactant mixture with an equivalence ratio of about 0.8. This is because even for the combustion of the stoichiometric mixture, some incomplete products of combustion are formed.

Fig. 11 Percentage availability destroyed and product mixture temperature as functions of equivalence ratio for constant volume combustion of iso-octane for a reactant pressure of 500 kPa and a reactant temperature of 300 K

3.3 Constant temperature combustion process

In addition to constant pressure and constant volume combustion processes, constant temperature combustion processes were also studied. For cases of constant temperature, either the pressure or the volume of the system also needs to be fixed to allow the system to be fully defined. Both isobaric and isochoric constant temperature combustion processes were studied. To maintain a constant temperature, thermal energy (and the associated availability) must be moved across the system boundary during the combustion process. This thermal energy (availability) can be further utilized to do work in a heat engine and is, therefore, included in the availability balance (equations (12), (16), (18), and (20)). Note that the approach adopted here distinguishes between the destruction due to combustion and the availability that is 'moved' with the heat transfer.

Figure 12 shows the percentage availability destroyed during the combustion process for an isobaric, constant temperature combustion process as functions of temperature for reactant pressures of 50, 500, and 5000 kPa. Initially, at low temperatures, almost the entire reactant availability is destroyed. This is because the energy associated with heat transfer at 298.15 K has no potential to do work and, therefore, the entire chemical energy present in the fuel is destroyed by converting the reactants to products at this low temperature. With increasing temperatures, the percentage of availability destroyed decreases. The effect of the reactant pressure on the percentage availability destroyed was once again relatively modest, with the percentage of availability destroyed due to combustion increasing with decreasing pressure.

Fig. 12 Percentage availability destroyed as functions of reactant temperature for three reactant pressures for constant temperature, isobaric combustion

The results for isochoric constant temperature combustion follow similar trends, and these results have been omitted here for conciseness, but are available elsewhere [12]. The only difference for the isochoric constant temperature combustion is that the curves for the various pressures would intersect because of the effect of the specific volume term in the availability, as described for the constant volume combustion process.

Figure 13 shows the variation in the percentage availability destroyed as functions of the temperature for equivalence ratios of 0.1, 0.5, and 1.0. The highest availability destruction is for reactant mixtures with an equivalence ratio of 1.0. For mixtures with lower (leaner) equivalence ratios, the destruction of availability decreases. This is because conversion of the reactants into products for the stoichiometric mixture liberates the greatest amount of energy. As the temperature of the system is maintained constant in this combustion process, this energy is transferred across the system boundary as heat transfer. This heat energy is not entirely available, with the available fraction of this energy being determined by the expression for Carnot efficiency. As a consequence, the combustion of the stoichiometric mixture with greater heat transfer results in the greatest percentage destruction of availability.

Figure 14 shows similar results for the percentage availability destroyed as functions of temperature for equivalence ratios of 1.0, 1.5, and 2.0. At lower temperatures (<2000 K), the percentage availability destroyed is greatest for the equivalence ratio of 1.0, decreasing with increasing equivalence ratios.

Fig. 13 Percentage availability destroyed as functions of reactant temperature for three lean equivalence ratios for constant temperature, isobaric combustion of iso-octane for a reactant pressure of 500 kPa

For temperatures >2500 K, these values converge. Once again, the availability balance was conducted after accounting for the reactive availability of the product mixture. If this is not accounted for, the trend would change, with the least destruction of availability occurring for the stoichiometric reactant mixture.

Figures 13 and 14 show the results for isobaric constant temperature combustion. The results for isochoric constant temperature combustion show similar trends and, therefore, have not been presented in this work, but may be found in reference [12].

3.4 Comparison of results for various combustion processes

The preceding sections have examined the effect of the various parameters on the destruction of availability due to combustion for the different combustion processes. Figure 15 shows a comparison between the constant pressure and the constant volume combustion processes for reactant pressures of 50, 500, and 5000 kPa. For a reactant pressure of 50 kPa, the curves for the percentage availability destroyed during constant pressure and constant volume combustion do not intersect, with the destruction of availability being consistently lower for the case of constant volume combustion. For higher reactant pressures of 500 and 5000 kPa, the curves for the percentage availability destroyed during constant pressure and constant volume combustion intersect for a reactant temperature of ~ 1000 K. For reactant temperatures greater than ~ 1000 K, the percentage availability destroyed is

Fig. 14 Percentage availability destroyed as functions of reactant temperature for three rich equivalence ratios for constant temperature, isobaric combustion of iso-octane for a reactant pressure of 500 kPa

Fig. 15 Comparison of constant pressure and constant volume combustion processes for three reactant pressures

greater for the constant volume combustion process, whereas for lower temperatures, the percentage availability destroyed is greater for constant pressure combustion process. Also, although the trends for reactant pressures of 500 and 5000 kPa are similar, the magnitudes of the percentage availability destroyed due to the combustion processes are lower for the case of reactant pressure of 5000 kPa, in accordance with previous results.

Figure 16 shows a comparison between the constant pressure and constant volume combustion processes for equivalence ratios of 0.10, 1.00, and 2.00. For an equivalence ratio of 0.10, the constant volume combustion process destroys a larger percentage of the reactant availability, throughout the temperature range examined. For equivalence ratios of 1.00 and 2.00, the curves for the percentage availability destroyed due to constant pressure and constant volume combustion processes intersect, indicating that for these equivalence ratios, the destruction of availability is greater for the constant pressure combustion process at low temperatures and greater for the constant volume combustion process at higher temperatures.

Figure 17 shows the percentage availability destroyed due to constant pressure, constant volume, and constant temperature (and isobaric) combustion processes as functions of reactant temperature for a reactant pressure of 500 kPa and equivalence ratio of 1.0. The percentage availability destroyed due to combustion decreased with increasing reactant temperatures for all three combustion processes examined. Initially, for low temperatures (less than ~ 2000 K), the percentage availability destroyed due to the constant temperature combustion process is significantly higher than that for the constant pressure and constant volume

Fig. 16 Comparison of constant pressure and constant volume combustion processes for three equivalence ratios

combustion processes. This is because conversion of reactants into the products at fixed low temperatures destroys most of the reactant availability.

3.5 Discussion and comparison to previous work

As indicated previously, Dunbar and Lior [4] have completed an analysis of constant pressure combustion processes with hydrogen and methane as the fuels. The results from the current work were compared with the results for the overall destruction of availability during the combustion process for hydrogen. The value obtained during the analysis by Dunbar and Lior [4] for the destruction of availability due to combustion of hydrogen at 298 K and atmospheric pressure is ~ 54 MJ/kmol- H_2 , whereas

Fig. 17 Comparison of constant pressure, constant volume, constant temperature isobaric combustion processes for reactant pressure of 500 kPa and equivalence ratio of 1.0

the value computed from the current work is ~ 53.9 MJ/kmol- H_2 . These calculations are based on slightly different conditions than for the present work. For example, Dunbar and Lior [4] assumed the atmospheric composition to be 79 per cent nitrogen and 21 per cent oxygen. This composition is different from that assumed in the current analysis, but does not have a significant impact on the destruction of availability.

The results for the constant volume combustion process from the current study were also compared with the results from the analysis conducted by Caton [5]. The values of the product mixture temperature, product mixture pressure, and the percentage availability destroyed were compared. Again, the trends were in agreement, but the absolute values were slightly different. This was because for combustion, the current analysis used a 'wet' air (Table 1) whereas Caton [5] used a dry air. In addition, the current analysis uses a newer set of coefficients for determining the thermodynamic data.

In addition, the current results were also compared with the results from the analysis completed by Daw *et al.* [6] for constant pressure combustion processes. The current work examines unconstrained combustion of the fuels in air, whereas the work by Daw *et al.* [6] examined a modified hypothetical isobaric combustion process, which they refer to as counter-flow preheating with equilibrium reaction. The values for the availability efficiency themselves could not be compared. The values of peak flue gas temperatures, however, were compared and were in agreement with each other.

3.6 Importance of chemical availability

A rigorous implementation of the chemical availability component was completed and the relative contribution of the various availability terms was examined. The contribution of the diffusion availability term was insignificant, whereas the thermo-mechanical availability and the reactive availability terms were significant. The detailed results that support these statements are presented in Appendix 1.

3.7 Effect of reactant mixture dissociation

The decrease in the percentage of reactant availability destroyed due to combustion at higher reactant temperatures tends to suggest the possibility of reversible combustion for high reactant temperatures. This trend, however, neglects to consider the effects of reactant mixture dissociation. Once the effects of the reactant mixture dissociation are included, the percentage availability destroyed values are lower than the case without reactant mixture dissociation. This effect is examined in more

detail in Appendix 2. Combustion losses would be reduced if the reactant mixture were preheated to this temperature before the combustion process.

4 SUMMARY AND CONCLUSIONS

A parametric examination of the availability destroyed during combustion of iso-octane and air mixture was completed for constant pressure, constant volume, and constant temperature combustion processes. The effect of the reactant mixture temperature, pressure, and equivalence ratio on the percentage of availability destroyed due to the combustion processes was determined. The results are summarized as follows.

1. The effect of the reactant mixture temperature on the percentage of availability destroyed during the combustion processes was most significant when compared with the other parameters. For typical conditions, the percentage of availability destroyed decreased from ~30 per cent for reactant temperatures of 300 K to ~5 per cent for reactant temperatures of 4500 K for constant pressure and constant volume combustion processes. A similar trend was observed for constant temperature combustion. The magnitudes of the values of the percentage of availability destroyed due to constant temperature are, however, different on account of the difference in the combustion process resulting from the imposed temperature restraint. This decrease in the percentage availability destroyed with increasing reactant temperatures is consistent with the decreased availability associated with combustion at higher temperatures, as documented previously by a number of authors [4–6].
2. The effect of the reactant mixture pressure on the percentage of availability destroyed due to combustion was examined and was noted to be modest in comparison to the effect of the reactant mixture temperature for the different combustion processes. For reactant pressures ranging from 50 to 5000 kPa, the variation in the percentage availability destroyed due to combustion was noted to be <5 per cent (of the total reactant mixture availability).
3. The effect of the reactant mixture equivalence ratio was also examined, and it was found that the percentage destruction of availability decreased monotonically with increasing equivalence ratios. By neglecting the reactive availability of the products, the percentage destruction of availability increased for richer mixtures. This reflects the fact that most of the reactant availability in rich mixtures is not converted into

thermo-mechanical availability during the combustion process, but is preserved as the chemical energy of the incomplete products of combustion. Therefore, the least destruction of availability corresponds to combustion of near stoichiometric mixtures.

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APPENDIX 1

Importance of chemical availability

This section examines the contribution and the relative significance of the various components for the availability of a system. The three components examined are the thermo-mechanical, reactive, and the diffusion availability. Again, the mixtures examined are iso-octane vapour and air.

Figure 18 shows the reactant availability components as functions of reactant mixture temperature for a reactant pressure of 500 kPa and an equivalence ratio of 1.0. As expected, at 300 K, the contribution of the thermo-mechanical availability to the total availability is negligible. This term monotonically continues to increase, however, with increasing temperature. The reactive availability term, due to the chemical energy of the fuel, is independent of the temperature and remains constant. The diffusion availability is also fixed in magnitude, but is much smaller in value and overall significance.

Figure 19 shows the product availability components as functions of product temperature. At 300 K, all three components of the availability are small in magnitude. The thermo-mechanical availability increases with increasing temperature and is dominant until ~2500 K. At temperatures >2500 K, the increased presence of incomplete products of combustion contributes to the reactive availability

Fig. 18 Various components of the total reactant mixture availability for stoichiometric mixture of iso-octane for a reactant pressure of 500 kPa and an equivalence ratio of 1.0

Fig. 19 Various components of the total product mixture availability for stoichiometric mixture of iso-octane for a product pressure of 500 kPa and an equivalence ratio of 1.0

term and consequently, this term rises sharply. The diffusion availability component is fixed in magnitude and is once again, not significant compared to the total mixture availability.

In summary, the diffusion availability component is not of much significance as compared to the total mixture availability and may be neglected without significant loss in accuracy of the computation, as pointed out by a number of authors [1, 2]. The reactive availability of the mixtures, however, cannot be neglected and under some conditions, is more significant than even the thermo-mechanical availability of the mixture.

APPENDIX 2

Effect of reactant mixture dissociation

At some of the higher reactant mixture temperatures discussed in this work, past 3000 K, the reactant mixture species are no longer stable and tend to dissociate. This dissociation needs to be accounted for in the availability analysis to obtain a more complete understanding of the combustion processes. In this determination, the various species were allowed to dissociate independently of each other, i.e. the various reactant mixture species did not react with each other. The species considered for this dissociation process are H_2 , H , OH , H_2O , O_2 , O , Ar , N_2 , N , CO_2 , CO , CH_4 , C_2H_2 , C , C_2 , C_3 , and CH . For the purpose of this analysis, it was assumed that carbon exists as a gas. This is true for temperatures greater than ~4300 K. For lower temperatures, this assumption would lead to some level, though not significant, of approximation.

Fig. 20 Effect of reactant mixture dissociation on reactant availability

Figure 20 shows the reactant mixture availability with and without the reactant mixture dissociation being considered. For temperatures greater than ~ 3000 K, the effect of the reactant mixture dissociation is significant. The increased availability of the dissociated reactant mixture is due to the fact that the dissociated reactant mixture possesses greater energy, absorbed during the process of breaking the chemical bonds of the various species. The

Fig. 21 Percentage availability destroyed during constant volume combustion of iso-octane for reactant pressure of 500 kPa, with and without reactant mixture dissociation

Fig. 22 Product mixture temperature as a function of reactant mixture temperature, with and without reactant mixture dissociation for constant volume combustion of iso-octane, reactant pressure 500 kPa

initial difference between the two curves at lower temperatures (< 3000 K) is due to the fact that the equilibrium prediction of iso-octane is that it decomposes into methane, hydrogen, and carbon. This decomposition is not realistic since, at low temperatures, the chemical kinetics are expected to be too slow for this to be observed. (The current work did not include any chemical kinetics). For more stable fuels such as hydrogen and methane, these curves were found to overlap at these lower temperatures.

Figure 21 shows the percentage availability destroyed for a constant volume combustion process, with and without considering the effects of the reactant mixture dissociation. The two curves are nearly parallel to each other (again, the difference between the two cases is due to the equilibrium products predicted for iso-octane) with lower destruction of availability for the case with reactant mixture dissociation considered.

Figure 22 shows the product mixture temperatures with and without considering the effect of the reactant mixture dissociation. Without considering the effects of the reactant mixture dissociation, it is found that at temperatures past 3500 K, the combustion process would be endothermic. This is not true, however, and the curve for the product mixture temperature considering the effect of reactant mixture dissociation rises sharply, and the combustion process is exothermic once this effect is accounted for in the analysis.