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Implications of fuel selection for an SI engine: Results from the first and second laws of thermodynamics

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ABSTRACT

The current work examines the detailed thermodynamics of the use of eight (8) fuels by an automotive, spark-ignition engine using a thermodynamic engine cycle simulation. The fuels examined were methane, propane, hexane, isooctane, methanol, ethanol, carbon monoxide, and hydrogen. Both overall engine performance parameters and detailed instantaneous quantities are determined for each of the fuels. Results include thermal efficiencies, heat transfer, and exhaust gas temperatures as functions of engine speed and load. In general, the overall engine results were similar for the various fuels. The second law results showed that, for the same operating conditions, the destruction of exergy during the combustion process ranged between about 8% (for carbon monoxide) and 21% (for isooctane) of the fuel exergy depending on the specific fuel. The differences of the exergy destruction during combustion appear to be related to the complexity of the fuel molecule and the presence (or lack) of oxygen atoms in the fuel molecule.

1. Introduction

The use of various fuels for internal combustion engines began as early as the late 1800s during the development of the first IC engines [1–4]. Over the years, these fuels have included gasoline, diesel, natural gas, liquefied petroleum gas (LPG), other fuel gases, alcohols, and numerous other gaseous and liquid fuels. Each of these fuels has advantages and disadvantages. Often the fuel is considered for IC engines when it is a more economical choice than the current fuel. Also, in recent years, fuels that possess naturally lower emissions are often considered as replacements for more conventional petroleum fuels.

Gasoline and diesel have been the conventional fuels for spark-ignited and compression-ignited engines since the 1900s. Over the years these two fuels have been and continue to be modified to provide the performance characteristics that are required [1,2]. As stated elsewhere, the success of IC engines has been at least in part due to the excellent match of conventional fuels and engines [1–3].

The literature on fuels for engines is vast. These previous studies range from economic assessments [5] to technical evaluations [6]. In addition to the literature cited above, other examples of previous technical work include examinations of the autoignition characteristics of alcohol fuels [7] and evaluations of blends of gaseous fuels [8]. No single reference was found which included the eight fuels of the current study, and no work appears to have completed a consistent thermodynamic evaluation of a set of fuels.

The objectives of the current work (using an engine cycle simulation) are to compare the performance and second law parameters of a conventional spark-ignition engine operated on each of eight (8) fuels: methane, propane, hexane, isooctane, methanol, ethanol, carbon monoxide, and hydrogen. The comparisons are completed for a base case part-load condition, and as functions of speed and load.

2. Engine cycle simulation description

The cycle simulation used in this work has been described in detail elsewhere [9–12]. This simulation is largely based on thermodynamic formulations, and is a complete representation of the four-stroke cycle including the intake, compression, combustion, expansion and exhaust processes. The simulation uses detailed thermodynamic gas properties including equilibrium composition for the burned gases. The cylinder heat transfer is adopted from the correlation by Woschni [13], and the combustion process is based on a mass fraction burn relation from Wiebe [14]. The major assumptions and approximations used in the development include the following:

(1) the thermodynamic system is the cylinder contents (see Fig. 1)

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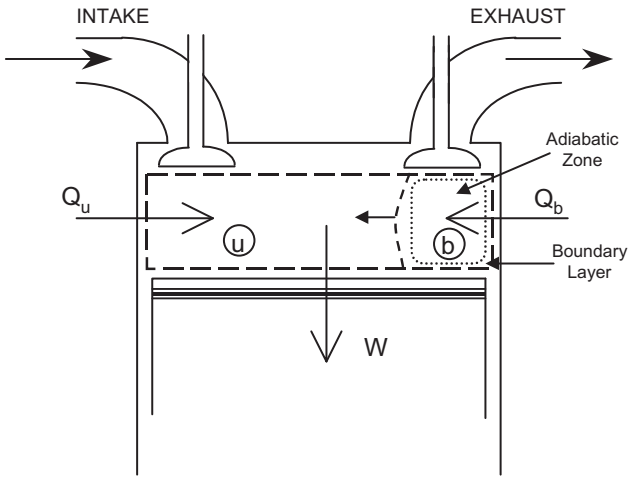

Fig. 1. Schematic of the engine cylinder and the thermodynamic system.

(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. The total heat transfer is divided in an appropriate fashion between the unburned and burned zone. The heat transfer from the burned zone is assigned in total to the boundary zone [9,10]
(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 [15] and the species obey the ideal gas equation of state
(8) the instantaneous thermodynamic properties are computed from established formulations [15] 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 [15]
(10) the fuel is completely vaporized in the intake ports and mixed with the in-coming air
(11) the combustion efficiency is 99.3% (a result of the selected Wiebe constants)
(12) the blow-by is zero

Other assumptions and constraints apply to the results of this study. For example, combustion stability, cycle-to-cycle variations, or other combustion issues are not included. Further, knock, preignition, or other abnormal combustion phenomena are not considered. Again, the focus of the work is to compare and contrast the fuels from a thermodynamic perspective and not to describe the details of the combustion process. More detailed simulations (e.g., using CFD) would provide more information on the combustion process, but the results would conform with the thermodynamics.

The majority of the above assumptions and approximations have been validated and used in a number of previous simulations. Although no experimental data are cited in the current paper, previous work [15,16] has demonstrated the success of these types of simulations for duplicating experimental results.

2.1. Energy equations

As a result of the thermodynamic analysis, governing differential equations are obtained for the gas temperatures, the cylinder pressure, the volumes, and the masses. 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. An Euler technique was selected for the numerical integration of these equations.

For the one zone cases, the following is the appropriate relation:

$$\frac{d(mu)}{d\theta} = \dot{Q} - pd\dot{V} + \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} \quad (1)$$

where m is the cylinder mass, u is the specific internal energy, θ is crank angle, $\dot{Q}$ is the rate of heat transfer, p is the cylinder pressure, $\dot{V}$ is the rate of cylinder volume change, $\dot{m}_{in}$ is the mass flow rate into the cylinder, h_{in} is the specific enthalpy of the inlet mixture, $\dot{m}_{out}$ is the mass flow rate out of the cylinder, and h_{out} is the specific enthalpy of the exiting mixture. This equation may be used to find an explicit relation for the derivative of the overall average cylinder gas temperature and cylinder pressure.

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

For the combustion process, multiple zones are used (see Fig. 1). First, the formulation is developed 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. The burned zone entrains mass from the unburned zone as the flame front proceeds.

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 initial values and the specified tolerance, this procedure usually finds convergence within about three (3) complete cycles.

2.2. Friction

The engine friction includes the mechanical friction and the pumping friction. The mechanical friction, in turn, includes the rubbing friction (such as from the crank, pistons, and valve train) and the work associated with the auxiliaries (such as oil and water pump, and alternator). Algorithms for each of these items were published by Sandoval and Heywood [17], and these are used here exactly as presented.

2.3. Exergy parameters

The exergy (or available energy) of the fuel and the cylinder gases is described by a number of parameters. For completeness, these parameters are briefly discussed next. Full details are available elsewhere [9–12].