PROPERTY DETERMINATION FOR ETHANOL-GASOLINE BLENDS WITH APPLICATION TO MASS FRACTION BURN ANALYSIS IN A SPARK IGNITION ENGINE

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Abstract

The Mass Fraction Burn (MFB) and Heat Release Rate (HRR) reflects the amount of fuel burned, and the rate of burning throughout the combustion process in an internal combustion engine. These parameters play a crucial role in research and development endeavors focused on engine efficiency, emissions, and overall operating performance. They are computed by analyzing measured pressure data and applying thermodynamic principals to determine the energy released during the combustion process. Thus, the properties of the fuel-air and combusted gas mixtures play an important role in the analysis.

Engine pressure data were taken from a Spark-Ignition Cooperative Fuels Research (CFR) engine operating at a constant load of 330 kPa Net Indicated Mean Effective Pressure (Net IMEP) and using five ethanol-gasoline fuel blends: E0 (gasoline), E20, E40, E60, and E84. The fuels were assumed to be in a non-reacting state throughout the mixing process. Once the fuel mixture properties were known, the fuel-air and burned mixture properties were determined using the fuel-air mass ratio. The analysis presented within this paper details the process by which the fuel, fuel-air, and burned mixture properties can be determined. The MFB of five different fuel blends at a chosen operating condition was also presented along with the pressure trace, the temperature and the gamma profile at the end of this paper.

Keywords: *ethanol-gasoline blend, mass fraction burn, heat release, IC engine, fuel-air mixture properties*

1. Introduction

Properties of species that are involved in engine combustion as a function of temperature can be found in JANAF thermochemical data tables [1]. However, the properties of the mixture of particular species is not readily available. Newhall and Starkman [2] developed the thermodynamic properties charts of burned and unburned mixtures of octane and air. Later, Olikara and Borman [3] developed a computer program to calculate the properties of products based on equilibrium combustion. Both of these works started the calculation based on mole fraction and returned results on a mass basis for application to IC engine calculations. Investigation of the thermodynamic properties of ethanol and gasoline blends in this research started from the concept of blending the fuels and then moved to the concept of mixing between the air, fuels and the products of the combustion. This included the calculation of gamma. Gamma is the ratio of the constant pressure specific heat to the constant volume specific heat which depends on the fuel and air mixture conditions and plays an important role in the further analysis of the combustion process in IC engines.

Mass fraction burned as a function of crank angle represents the percentage of fuel consumed versus crank angle during the combustion process in an engine cycle. It shows that the rate at which the fuel-air mixture burns increases after the spark discharge to a maximum about halfway through the burning process and then decreases to zero as the combustion process ends. The mass fraction burned curve, which has a characteristic S-shape, is commonly used to characterize and develop the combustion process. A single-zone model has been developed and compared with a two-zone model using ethanol-gasoline fuel blends in a CFR engine [4]. Derived from the energy balance and the ideal gas equations, the single-zone model, with two unknowns (temperature and mass fraction burn), is proven to correlate well with the two-zone model, particularly in regards to combustion phasing. In this work, the mass fraction burn is calculated from experimental data using the single-zone model.

2. Experimental Setup

A single cylinder CFR engine, (manufactured by the Waukesha Motor Company), was used to generate the data used in this research. Several modifications have been incorporated to meet the criteria for this research. The experiments were conducted by sweeping ethanol concentration, spark timing and compression ratio at constant engine speed and a constant indicated load of 330 kPa Net IMEP. The cylinder pressure data was obtained with an AVL GH12D piezoelectric pressure transducer. Data acquisition, including the measurement of cylinder pressure and various other critical pressures and temperatures, was accomplished using a combination of National Instruments (NI) hardware and software. A control system for this CFR engine had been previously developed by Naber, et al. [5], with Mototron's Motohawk rapid engine control development environment. Mototron's Mototune was used as the calibration tool and ECU interface. The calibration tool was also used to record engine control parameters such as intake manifold pressure, air flow rate, spark timing, fuel injection pressure, injection duration, commanded equivalence ratio, etc.

3. Composite Fuel

Assuming an ideal, non-reacting mixing process, the formation of one mole of total fuel blend is expressed as:

$$\left(1-\overline{E}\right)\left(CH_{\beta}O_{z}\right)_{\alpha}\Big|_{gasoline}+\overline{E}\left(CH_{\beta}O_{z}\right)_{\alpha}\Big|_{ethanol}=\left(CH_{\beta*}O_{z*}\right)_{\alpha*}. \tag{1}$$

The indexies of the composite fuel can be obtained as follow:

$$\alpha*=\left(1-\overline{E}\right)\cdot\alpha_{gasoline}+\left(\overline{E}\right)\cdot\alpha_{ethanol}\,, \tag{2}$$

$$\beta*=\frac{\left(1-\overline{E}\right)\cdot\beta_{gasoline}\cdot\alpha_{gasoline}+\left(\overline{E}\right)\cdot\beta_{ethanol}\cdot\alpha_{ethanol}}{\left(1-\overline{E}\right)\cdot\alpha_{gasoline}+\left(\overline{E}\right)\cdot\alpha_{ethanol}}, \tag{3}$$

$$z*=\frac{\left(1-\overline{E}\right)\cdot z_{gasoline}\cdot\alpha_{gasoline}+\left(\overline{E}\right)\cdot z_{ethanol}\cdot\alpha_{ethanol}}{\left(1-\overline{E}\right)\cdot\alpha_{gasoline}+\left(\overline{E}\right)\cdot\alpha_{ethanol}}. \tag{4}$$

Since gasoline is a refined petroleum product which consists of many hydrocarbons, given the molecular weight of 105 and the hydrogen to carbon ratio of 1.87, the averaged number of carbon atoms (equal to 7.56) can be calculated. Tab. 1 shows the composition of gasoline-ethanol mixtures in the $(CH_{\beta}O_z)_{\alpha}$ form. The α, β, and z for gasoline and ethanol data are taken from Heywood [6], while the α, β, and z for gasoline ethanol blends are calculated using the composite fuel concept using the given base fuel composition.

Tab. 1. Composition of gasoline-ethanol blends in the $(CH_\beta O_z)_\alpha$ form

	Gasoline	E20	E40	E60	E85	Ethanol
α	7.56	6.44	5.33	4.22	2.83	2.00
β	1.87	1.94	2.04	2.19	2.55	3.00
z	0.00	0.03	0.07	0.14	0.30	0.50

4. Combustion Reaction

Considering complete combustion, the reaction of a single mole of an oxygenated-hydrocarbon fuel can be expressed as follows:

$$\left(CH_\beta O_z\right)_\alpha + \alpha\frac{A_s - z/2}{\phi}\left(O_2 + \psi N_2\right) = n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{N_2}N_2 + n_{O_2}O_2 + n_{CO}CO + n_{H_2}H_2, \quad (5)$$

$$\alpha = \frac{MW_f}{12.011 + 1.008\cdot\beta + 16.00\cdot z}, \quad (6)$$

$$A_s = 1 + \frac{\beta}{4}, \quad (7)$$

The reactant and product compositions of one mole of oxygenated-hydrocarbon fuel reacted with air is summarized in Tab. A1 (appendix). For a fuel-rich mixture, the water gas shift reaction constant is assumed to be a function of temperature, and there is no oxygen in the products. For a fuel-lean mixture, carbon monoxide and hydrogen are assumed not present in the products [6]. The ratio of the number of moles of products to reactants does not vary significantly with respect to the ethanol concentration, as shown in Fig. 1a. However, the total number of moles of reactants and products decreases significantly with higher ethanol content, particularly in the lean condition, as shown in Fig. 1b. The inflection point that marks the stoichiometric reaction is caused by the difference in the rich and lean composition assumptions.

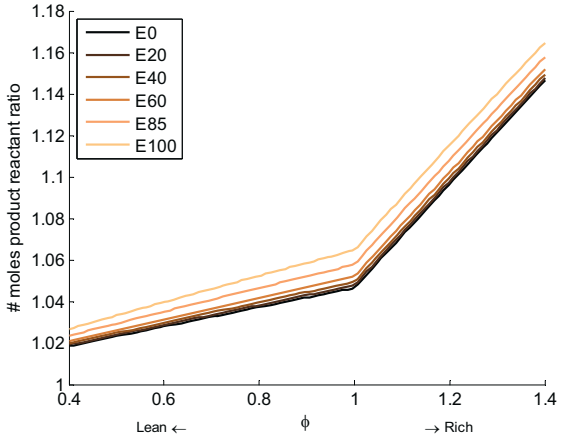


Fig. 1a. Ratio of number of moles of products to reactants of gasoline-ethanol blends as function of equivalence ratio based one mole of fuel

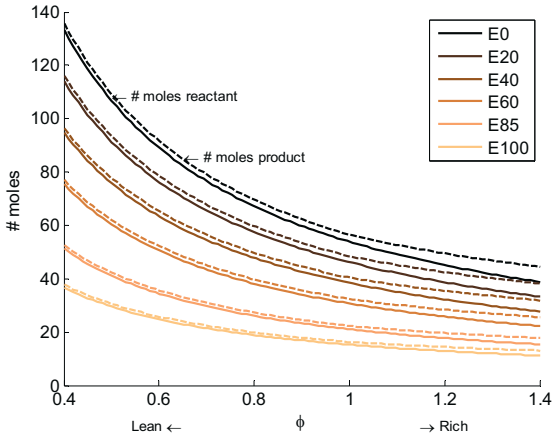


Fig. 1b. Number of moles of products and reactants of gasoline-ethanol blends as function of equivalence ratio based one mole of fuel

The number of moles of reactant and product for stoichiometric combustion can be expressed:

$$\frac{\#\ moles\ products}{\#\ moles\ reactans} = \frac{\alpha + \alpha\ \beta/2 + \alpha\,\psi\left(1+\beta/4 - z/2\right)}{1+\alpha\left(1+\beta/4 - z/2\right)\left(1+\psi\right)}. \tag{8}$$

Tab. 2 shows the number of moles of reactant and product for stoichiometric combustion of the blended fuel in this research.

Tab. 2. Ratio of number of moles of products to reactants of gasoline-ethanol blends at stoichiometric condition

	Gasoline	E20	E40	E60	E85	Ethanol
#moles products	56.46	48.43	40.39	32.36	22.32	16.29
#moles reactants	53.93	46.20	38.47	30.75	21.09	15.30
#moles products/#moles reactants	1.05	1.05	1.05	1.05	1.06	1.07

5. Lower Heating Value

Using the fuel compositions provided in Tab. 1, the molecular weight of the composite fuel is:

$$MW_f = \alpha\left(12.011 + 1.008\cdot\beta + 16.00\cdot z\right). \tag{9}$$

The lower heating value of the blended fuel mixture on a molar basis is expressed as:

$$\overline{LHV}_f = \left(1-\overline{E}\right)\cdot\overline{LHV}_{gasoline} + \left(\overline{E}\right)\cdot\overline{LHV}_{ethanol}. \tag{10}$$

The lower heating value of the blended fuel mixture on a mass basis is expressed as:

$$LHV_f = \frac{\overline{LHV}_f}{MW_f}. \tag{11}$$

6. Air Fuel Ratio

The air fuel ratio to completely burn the blended fuel can be calculated from equation 12 below, where the number of moles of oxygen and nitrogen are given in Tab. A1:

$$AFR = \frac{n_{O_2}\cdot MW_{O_2} + n_{N_2}\cdot MW_{N_2}}{n_f\cdot MW_f}. \tag{12}$$

Tab. 3 shows the molecular weight, lower heating value and the stoichiometric air fuel ratio of the blended fuels in this research.

Tab. 3. The molecular weight, the lower heating value and the stoichiometric air fuel ratio of gasoline-ethanol mixture using composite fuel calculation

	Gasoline	E20	E40	E60	E85	Ethanol
MW_f	105.00	93.20	81.40	69.60	54.85	46.00
LHV (MJ/kg)	43.46	41.83	39.72	36.90	31.66	26.90
AFR	14.54	13.99	13.28	12.33	10.56	8.96

7. Molecular Weight - Reactants and Products

Based on the composite fuel and combustion reaction calculation given in Tab. 1 and Tab. A1, the molecular weight of an oxygenated-hydrocarbon-air reactant mixture is calculated as:

$$MW_u = \frac{n_f \cdot MW_f + n_{o_2} \cdot MW_{o_2} + n_{N_2} \cdot MW_{N_2}}{n_u}, \tag{13}$$

And the molecular weight of the combustion products mixture is calculated as:

$$MW_b = \frac{n_{CO_2} \cdot MW_{CO_2} + n_{CO} \cdot MW_{CO} + n_{H_2O} \cdot MW_{H_2O} + n_{O_2} \cdot MW_{O_2} + n_{N_2} \cdot MW_{N_2} + n_{H_2} \cdot MW_{H_2}}{n_b}, \tag{14}$$

Tab. 4. The stoichiometric unburned and burned molecular weight of a gasoline-ethanol air reaction

	Gasoline	E20	E40	E60	E85	Ethanol
MW_u	30.25	30.23	30.20	30.16	30.07	29.96
MW_b	28.89	28.84	28.77	28.66	28.41	28.12

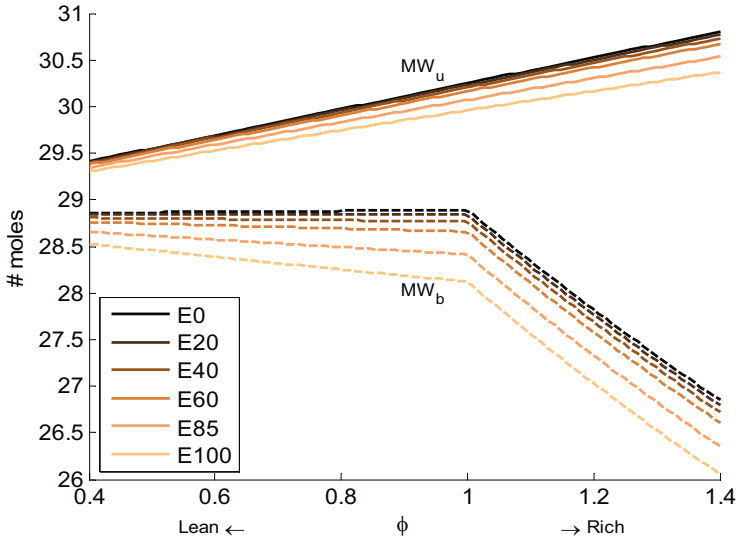


Fig. 2. Molecular weight of unburned and burned of gasoline-ethanol blends-air mixture as function of equivalence ratio

Fig. 2 shows the unburned molecular weight of gasoline-ethanol blends in mixture with air and the burned molecular weight of gasoline-ethanol blends after complete combustion. Due to the different assumption for products for rich and lean mixture, the molecular weight of the burned mixture has an inflection point at an equivalence ratio equal to one. The effect of ethanol concentration is more pronounced in the burned portion than in the unburned portion. Tab. 4 shows the unburned and burned molecular weight corresponding to the fuel blends used in this work for a stoichiometric reaction.

8. Gamma (Specific Heat Ratio)

The gamma of the fuel mixture can be derived from the constant pressure heat capacity data that is widely available for ethanol and gasoline [6]. Similarly, for the unburned and burned mixtures, gamma is calculated based on each species. The constant pressure heat capacity of those species can be found in Heywood [6]. The constant pressure specific heat capacity for the blended fuel mixture expressed on a molar basis is given by:

$$\overline{C}p_f = \left(1-\overline{E}\right)\cdot \overline{C}p_{gasoline} + \left(\overline{E}\right)\cdot \overline{C}p_{ethanol}. \tag{15}$$

The constant pressure specific heat capacity of an oxygenated-hydrocarbon-air reactant mixture that represents the unburned composition will be:

$$\overline{C}p_u = \frac{n_f \cdot \overline{C}p_f + n_{O_2} \cdot \overline{C}p_{O_2} + n_{N_2} \cdot \overline{C}p_{N_2}}{n_u}. \tag{16}$$

Similarly, the constant pressure specific heat capacity of the combustion products will be:

$$\overline{C}p_b = \frac{n_{CO_2} \cdot \overline{C}p_{CO_2} + n_{CO} \cdot \overline{C}p_{CO} + n_{H_2O} \cdot \overline{C}p_{H_2O} + n_{O_2} \cdot \overline{C}p_{O_2} + n_{N_2} \cdot \overline{C}p_{N_2} + n_{H_2} \cdot \overline{C}p_{H_2}}{n_b}. \tag{17}$$

Gamma can be calculated equal to (C_p / (C_p-R)). Fig. 3a shows the unburned gamma of a gasoline-ethanol blend – air mixture as a function of temperature, and Fig. 3b shows the burned gamma assuming ideal combustion. Overall, the gamma decreases as the ethanol concentration increases, and as the temperature increases.

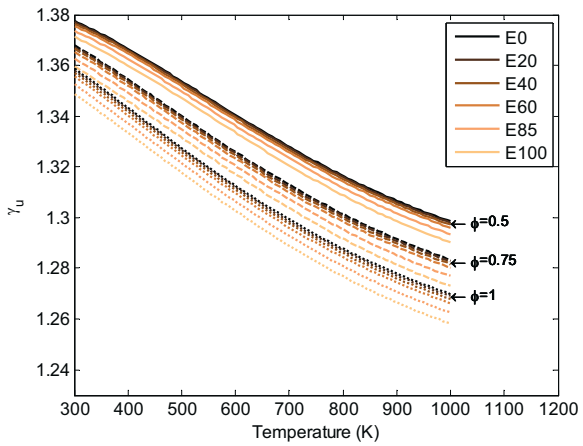


Fig. 3a. Gamma unburned of gasoline-ethanol blend-air mixture as a function of temperature

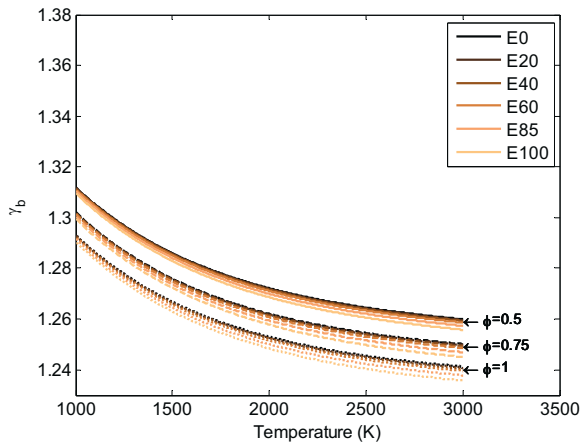


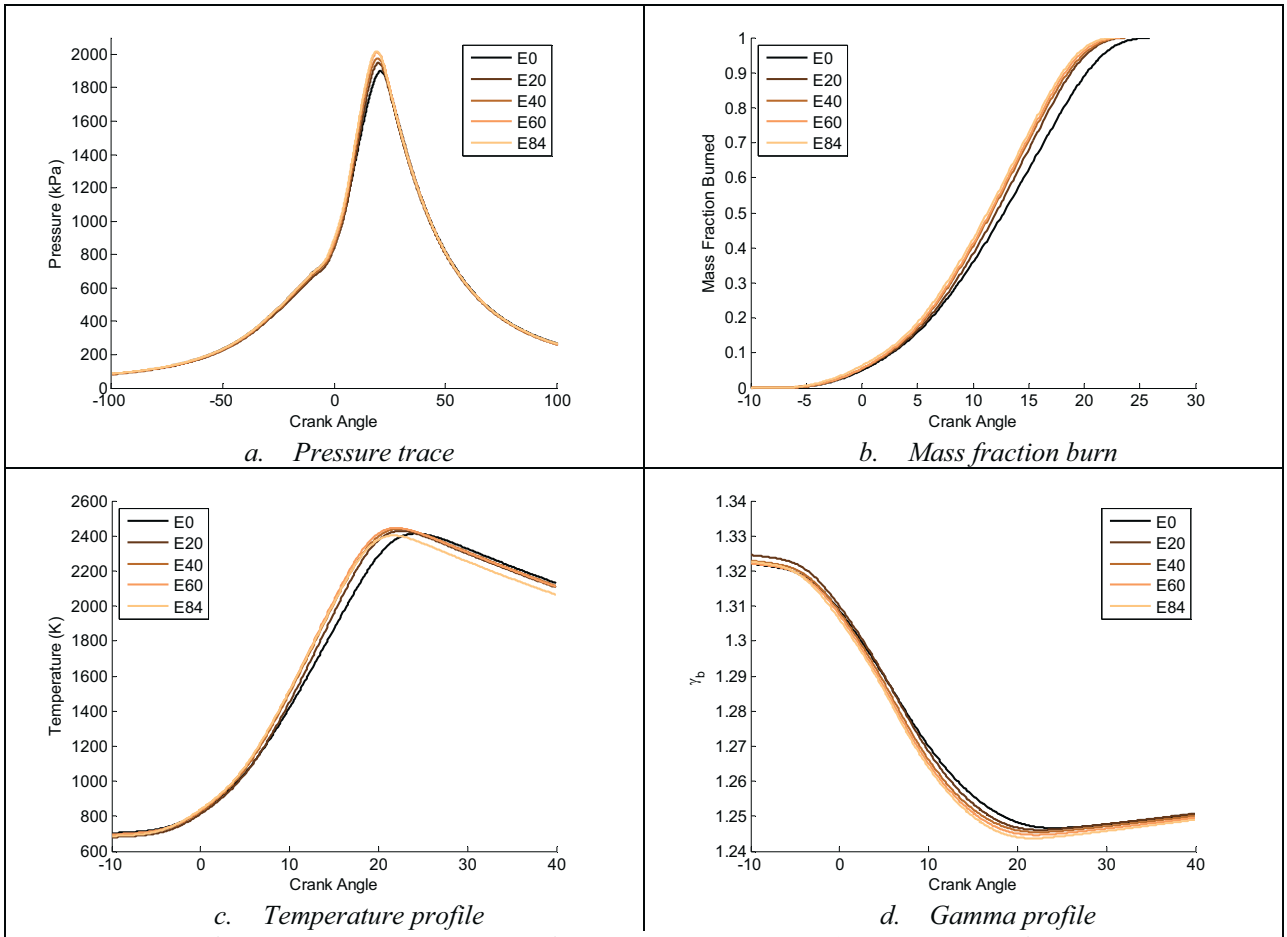
Fig. 3b. Gamma burned of gasoline-ethanol blend-air mixture as a function of temperature

Alternatively, the gamma of the burned mixture as a function of burned temperature and can be expressed by the following equation that covers stoichiometric combustion for all the fuel blends from E0 – E84 that have been used in this research with an error less than 0.18%. Using this equation simplifies subsequent fraction burned calculations.

$$\gamma_b = -0.0130\left(\frac{T_b}{1000}\right)^3 + 0.0880\left(\frac{T_b}{1000}\right)^2 - 0.2144\left(\frac{T_b}{1000}\right) + 1.4329. \quad (18)$$

9. Mass Fraction Burn Analysis

Fig. 4a shows the in-cylinder pressure trace in a CFR engine operating at a constant load and spark timing, for five different gasoline-ethanol fuel blends. Fig. 4b shows the mass fraction burn estimation using a single zone model, with the in-cylinder temperature profile and gamma as a function of temperature as inputs to the calculation. It is clearly shown that the mass fraction burn curve is a function of the pressure trace. The higher the ethanol content in the fuel blend, the higher the heat release rate, and thus the shorter the combustion duration. Fig. 4c shows the temperature profile, and Fig. 4d shows the gamma profiles starting from the point of ignition. The gamma decreases as the temperature increases. This trend, as well as the rank ordering of the different ethanol concentrations is consistent with the results shown in Fig. 3b.



a. Pressure trace *b. Mass fraction burn*

c. Temperature profile *d. Gamma profile*

Fig. 4. The Five different gasoline-ethanol blends using single zone mass fraction burn model (CFR engine, CR = 8.0:1, spark advanced = 10° BTDC, speed = 900 RPM, load = 330 kPa Net IMEP)

10. Conclusions

Several equations have been reviewed and introduced that can be used to calculate various thermodynamic propterties of blends of different fuels, fuel and air mixtures, and products of

combustion. Throughout this paper, these equations have been applied to the gasoline – ethanol blend ratios used in this research, and the results presented. Following are several conclusions that can be drawn from this work:

- the composite fuel concept that has been discussed in this paper is a simple and robust method for calculating various thermodynamic properties of fuel and fuel-air blends, as well as products of combustion,
- the number of moles of products and reactants is a function of both fuel composition as well as equivalence ratio,
- the Molecular Weight of the burned mixture is affected by ethanol concentration much more significantly than the molecular weight of the unburned mixture,
- the Molecular Weight of the burned mixture is a weak function of equivalence ratio for mixtures lean of stoichiometric, while it is a strong function of equivalence ratio for mixtures rich of stoichiometric,
- the gamma of both the unburned and burned mixtures are affected by variables such as ethanol concentration, equivalence ratio, and temperature. Except in the burned mixture, rich of stoichiometric, gamma tends to decrease with increasing ethanol concentration, and equivalence ratio. For burned mixtures rich of stoichiometric, gamma increases with increasing equivalence ratio,
- the properties of all species will affect the in-cylinder temperature profile calculation.

11. Nomenclature

$\bar{E}$	the volume percentage of ethanol in the ethanol - gasoline mixture,
α	number of carbon atoms in the fuel,
β	hydrogen to carbon ratio of the fuel,
z	oxygen to carbon ratio of the fuel,
A_s	stoichiometric moles of oxygen for hydrocarbon combustion,
ψ	nitrogen to oxygen ratio of the air,
ϕ	equivalence ratio,
MW_f	molecular weight of the fuel,
n	number of moles,
AFR	air fuel ratio,
LHV	lower heating value.

Subscripts

b	burned,
e	ethanol,
f	fuel,
g	gasoline,
u	unburned,
s	stochiometric reaction.

12. Acknowledgments

The authors would like to thank Craig Marriott and Matthew Wiles of GM Advanced Powertrain for their support, discussions, and feedback on this project.

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Appendix

Tab. A1. The gas composition of 1 mole of oxygenated-hydrocarbon fuel combusted with air

Unburned Composition	Burned Composition	
	$\phi \le 1$ (lean and stoic mixtures) CO and H_2 can be neglected	$\phi \ge 1$ (rich mixtures) O_2 can be neglected
$n_f = 1$ $n_{O_2} = \alpha \dfrac{A_s - z/2}{\phi}$ $n_{N_2} = \alpha \dfrac{A_s - z/2}{\phi}\psi$	$n_{CO_2} = \alpha$ $n_{H_2O} = 2\,\alpha\left(A_s - 1\right)$ $n_{N_2} = \alpha \dfrac{\psi\, A_s}{\phi}\left(1 - \dfrac{z}{2\,A_s}\right)$ $n_{O_2} = \alpha\, A_s \left(\dfrac{1}{\xi\phi} - 1\right)$ $n_{H_2} = 0$ $n_{CO} = 0$ $\xi = \dfrac{2}{\left(2 - \dfrac{z}{A_s}(1-\phi)\right)}$	$n_{CO_2} = \alpha\left(1 - n\right)$ $n_{H_2O} = \alpha\left(-d + 2\left(A_s - 1\right) + n\right)$ $n_{N_2} = \alpha \dfrac{\psi\, A_s}{\phi}\left(1 - \dfrac{z}{2\,A_s}\right)$ $n_{O_2} = 0$ $n_{H_2} = \alpha\left(d - n\right)$ $n_{CO} = \alpha\, n$ $n = \dfrac{-b \pm \sqrt{b^2 - 4\,ac}}{2\,a}$ $a = 1 - \kappa$ $b = 2\left(A_s - 1\right) + \kappa - d\left(1 - \kappa\right)$ $c = -\,d\,\kappa$ $d = 2\,A_s\left(1 - \dfrac{1}{\xi\phi}\right)$ $\kappa = \dfrac{n_{H_2O}\, n_{CO}}{n_{CO_2}\, n_{H_2}}$
$n_u = n_f + n_{O_2} + n_{N_2}$	$n_b = n_{CO_2} + n_{H_2O} + n_{N_2} + n_{O_2} + n_{H_2} + n_{CO}$	