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Steady-State Biodiesel Blend Estimation via a Wideband Oxygen Sensor

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\textbf{Abstract}—A substantial opportunity exists to reduce carbon dioxide (CO\textsubscript{2}) emissions as well as dependence on foreign oil by developing strategies to cleanly and efficiently use biodiesel, a renewable, domestically available, alternative diesel fuel. However, biodiesel utilization presents several challenges, including decreased fuel energy density and increased emissions of smog-generating nitrogen oxides (NO\textsubscript{x}). These negative aspects can be mitigated via closed-loop combustion control provided the properties of the fuel blend can be estimated accurately, on-vehicle, in real-time. To this end, this paper presents a method to practically estimate the biodiesel content of fuel being used in a diesel engine during steady-state operation. The simple, generalizable, physically motivated estimation strategy presented utilizes information from a wideband oxygen sensor in the engine’s exhaust stream, coupled with knowledge of the air-fuel ratio, to estimate the biodiesel content of the fuel. Experimental validation was performed on a 2007 Cummins 6.7 liter ISB series engine. Four fuel blends (0\%, 20\%, 50\% and 100\% biodiesel) were tested at a wide variety of torque-speed conditions. The estimation strategy correctly estimated the biodiesel content of the four fuel blends to within 4.2\% of the true biodiesel content. Blends of 0\%, 20\%, 50\% and 100\% were estimated to be 2.5\%, 17.1\%, 54.2\%, and 96.8\% respectively. The results indicate that the estimation strategy presented is capable of accurately estimating the biodiesel content in a diesel engine during steady-state engine operation. This method offers a practical alternative to in-the-fuel type sensors, because wideband oxygen sensors are already in widespread production and are in place on some modern diesel vehicles today.

\textbf{KEYWORDS}: biodiesel, diesel engines, alternative fuels, diesel fuel, biofuels, oxygenation, estimation, virtual sensing, fuel flexibility

\section{I. INTRODUCTION}

\textbf{A. Background}

Biodiesel is a renewable, alternative diesel fuel which can be produced from a wide variety of domestically available feedstocks. Vegetable oils and animal fats are reacted with an alcohol (typically methanol, although ethanol can also be used) in the presence of a catalyst to produce glycerin and fatty acid esters, which are commonly referred to as biodiesel. Biodiesel can be used in its pure form (B100), but is more commonly blended with conventional diesel fuel. Blends are designated BXX, where “XX” indicates the percentage of biodiesel by volume. B0 is conventional diesel. B5 is 5\% biodiesel, 95\% conventional. B20 is 20\% biodiesel, 80\% conventional, etc. Life cycle studies have shown that biodiesel contains substantially more energy than what is required for its production and also significantly reduces net carbon dioxide (CO\textsubscript{2}) emissions \cite{7},\cite{12} when produced from crops which consume CO\textsubscript{2} from the atmosphere. Biodiesel is also oxygenated, containing approximately 11\% oxygen by weight, generally believed to result in more complete combustion \cite{15} and thereby lower carbon monoxide (CO), unburned hydrocarbon (HC), and particulate matter (PM) emissions \cite{10},\cite{19}.

\textbf{B. Motivation}

Despite these benefits, the utilization of biodiesel also presents several challenges. The lower heating value of pure biodiesel is approximately 12\% less than that of conventional diesel \cite{15} and therefore a greater quantity of fuel is required to produce the same amount of power/torque. Another challenge is that unmodified engines using biodiesel typically emit higher levels of nitrogen oxides (NO\textsubscript{x}) \cite{15},\cite{14}. The “biodiesel NO\textsubscript{x} effect” has been, and continues to be, a subject of a great deal of scientific research where consensus for the exact reason(s) for this increase has not yet been reached \cite{3},\cite{9}. While increasing blends ratios of biodiesel generally results in dramatic decreases in particulate matter (PM), carbon monoxide (CO), and unburned hydrocarbon (HC), these reductions are frequently accompanied by increases in NO\textsubscript{x}.

A 2002 EPA study \cite{18} of pre-1998 model year engines showed that while emissions of PM, CO, and HC, were approximately cut in half for engines using B100, there was a 10\% increase in NO\textsubscript{x}. This may first appear to be an insignificant increase; however, EPA-mandated NO\textsubscript{x} emissions requirements have been some of the most difficult to meet, often requiring substantial increases in engine and aftertreatment complexity and cost. Therefore, any increase in NO\textsubscript{x} is met with significant concern and attention. Of even greater concern is the observation that these NO\textsubscript{x} increases appear to be more, and not less, dramatic in the most modern diesel engines \cite{5}, \cite{10}.

\begin{thebibliography}{9}

\end{thebibliography}
Many of the chemical and physical properties of biodiesel are different than those of conventional diesel. Important properties include cetane number, adiabatic flame temperature, density, lower heating value, viscosity, lubricity, and bulk modulus to name a few [15],[17],[14]. These “inputs” to the combustion process affect the “outputs”, namely of emissions, efficiency, and power. Research has shown that it may be possible to mitigate the negative aspects of biodiesel (namely higher NOx and reduced fuel economy) by active modulation of engine “actuators”, such as injection timing [13],[11], amount of exhaust gas recirculation (EGR) [2], and fuel injection pressure [4]. These parameters can be controlled on modern diesel engines through the engine control module (ECM). However, before strategies to accommodate the differences in the combustion behavior of different fuels can be practically implemented, a method must be developed to estimate the properties of the fuel being injected into the cylinder in real-time.

Estimating the percentage of biodiesel in the fuel blend will be a key enabler in allowing the ECM to maintain optimal engine performance across various fuel blends (B0 vs. B20 vs. B100, etc.). The objective of this paper is to examine the feasibility of using information from a production wideband oxygen (O2) sensor in the exhaust stream, coupled with knowledge of fuel and air flow, to estimate the biodiesel content in the fuel blend during steady-state engine operation.

C. Approaches Which Have Been Proposed by Others

Most of the research into the area of biodiesel blend sensing/estimation has focused on various types of sensors which would be emersed in the fuel (either in the fuel tank or in the fuel supply lines). Using refracor or dielectric based sensors has been suggested [16]. The use of other sensors which operate via near-infrared (NIR) spectroscopy or nuclear magnetic resonance (NMR) has also been proposed [8]. Others which utilize ultraviolet absorption spectroscopy [20] have also been proposed. Practical implementation of such sensors, however, presents several serious challenges. Most of these sensors would require a great deal of research and development before they could be inexpensively mass produced. Additionally, each engine/vehicle would require an additional sensor, something engine and vehicle manufacturers are reluctant to do because each additional sensor makes the engine/vehicle more complex and more costly to manufacture. Creatively using a wideband O2 sensor is attractive because it is an already established production sensor that, in some cases, is already installed on the vehicle for other purposes.

D. Fundamental Basis for Proposed Approach

Since biodiesel is an oxygenated fuel and conventional diesel is not, there are more oxygen atoms present in the cylinder prior to combustion for a given mixture fraction (mixture fraction is the mass fraction of fuel in the fuel-air mixture). Since the hydrogen/carbon atom ratio for conventional diesel and biodiesel are very similar, post combustion oxygen concentrations (oxygen left over after combustion) should theoretically be higher for biodiesel than conventional diesel. The hypothesis for this work is that the level of oxygen in the exhaust stream will be indicative of the percentage of biodiesel in the fuel blend, with the highest oxygen concentration expected for B100 and the lowest for B0. This provides a basis for developing a two-input, one-output biodiesel blend estimation strategy utilizing a wideband O2 sensor in the exhaust stream along with measurements/estimates of air and fuel flow as shown in Fig. 1.

![Fig. 1. Proposed Two-Input, One-Output Approach for Steady-State Biodiesel Blend Estimation](image)

The fundamental basis for this approach is essentially the same as what has been applied successfully in modern “fuel flexible” gasoline-ethanol vehicles. There are significant differences, however, in the operation of a conventional spark-ignited (SI) engine vs. the operation of a diesel engine which require that the same fundamental basis be applied in a different manner. In a conventional SI engine, an O2 sensor is present so that the exhaust oxygen concentrations can be maintained in a very narrow range where the air-fuel ratio is nearly stoichiometric (no excess fuel, no excess air). In a diesel engine, however, combustion is typically significantly lean of stoichiometric (i.e. excess air is present), and the air-fuel ratio undergoes very large fluctuations depending on operating conditions. If an O2 sensor is used in a diesel application it is typically used for determining the appropriate regeneration times for an oxygen-sensitive aftertreatment device such as a lean NOx trap. It is not being used for the purposes of maintaining the oxygen concentration within a particular range, as in an SI application. The combustion in diesel engines is typically also much more complete than in SI engines. The model which the proposed estimation strategy is based upon assumes lean, complete combustion to major products for the purposes of predicting exhaust O2 concentrations. That assumption is generally not a realistic assumption for SI engines.

II. THEORETICAL MODEL DEVELOPMENT

A. Prediction of O2 Levels for Different Blends

Combustion in diesel engines is significantly lean of stoichiometric and combustion inefficiency is $\leq 2\%$ [6], indicating essentially complete conversion of the fuel. Under these conditions, the global reaction of a generic oxygenated
hydrocarbon fuel ($C_nH_mO_r$) with idealized air ($O_2 + \epsilon N_2$) to major products ($CO_2$, $H_2O$, $O_2$, and $N_2$), is:

$$C_nH_mO_r + \lambda \left(n + \frac{m}{2} + \frac{r}{4} - \frac{\epsilon}{2}\right) (O_2 + \epsilon N_2) \rightarrow nCO_2 + \frac{m}{2}H_2O + \lambda (n + \frac{m}{4} - \epsilon) O_2 + \lambda \epsilon (n + \frac{m}{4} - \frac{r}{2}) N_2$$

where $n$, $m$, and $r$ are the number of carbon, hydrogen, and oxygen atoms in the fuel molecule, respectively. $\lambda$ is the excess air factor which is equal to the reciprocal of equivalence ratio (also equal to the actual air-fuel ratio divided by the stoichiometric air-fuel ratio) and $\epsilon$ is the mole ratio of nitrogen to oxygen in air.

The mixture fraction, $f$, is a function of the mass flow rate of air and the mass flow rate of fuel (both of which are controlled by the ECM in modern diesel engines). The mixture fraction is related to the air to fuel ratio (AFR) by:

$$f = \frac{\dot{m}_{fuel}}{\dot{m}_{fuel} + \dot{m}_{air}} = \frac{1}{1 + AFR}$$

The above definition can be applied to (1) to define the excess air factor, $\lambda$, in terms of the mixture fraction $f$:

$$\lambda = \left(\frac{1 - f}{f}\right) \left(\frac{n\alpha + m\beta + r\gamma}{n + \frac{m}{4} - \frac{\epsilon}{2}}\right)$$

where $\alpha$, $\beta$, and $\gamma$ are constants defined as:

$$\alpha = \frac{a_C}{2a_O + 2ca_N}, \quad \beta = \frac{a_H}{2a_O + 2ca_N}, \quad \gamma = \frac{a_O}{2a_O + 2ca_N}$$

with $a_C$, $a_H$, $a_O$, and $a_N$ representing the atomic masses of carbon, hydrogen, oxygen, and nitrogen, respectively. Substituting (3) back into (1) yields (4), the global reaction in terms of the mixture fraction.

$$C_nH_mO_r + \left(\frac{1-f}{f}\right) (n\alpha + m\beta + r\gamma) (O_2 + \epsilon N_2) \rightarrow nCO_2 + \frac{m}{2}H_2O + \epsilon (n\alpha + m\beta + r\gamma) N_2 + \left(\left(\frac{1-f}{f}\right) (n\alpha + m\beta + r\gamma) - n - \frac{m}{4} + \frac{r}{2}\right) O_2$$

Examination of (4) yields (5), the exhaust $O_2$ mole fraction.

$$x_{O_2} = \left(\frac{1-f}{f}\right) (n\alpha + m\beta + r\gamma) - n - \frac{m}{4} + \frac{r}{2}$$

Equation (5) captures the dependence of exhaust $O_2$ levels on the fuel’s molecular structure (via $n$, $m$, and $r$) and the proportions of air and fuel (via $f$). By definition, $n$, $m$, and $r$ for a biodiesel blend can be found via (6).

$$n = n_D + BD_{mol}(n_{BD} - n_D), \quad m = m_D + BD_{mol}(m_{BD} - m_D), \quad r = r_D + BD_{mol}(r_{BD} - r_D),$$

where the subscripts $D$ and $BD$ denote diesel and biodiesel, respectively. $BD_{mol}$ represents the biodiesel blend fraction on a molar basis (moles of biodiesel per total moles of fuel). Typically, however, the biodiesel blend is not known on a molar basis, but rather, on a volumetric basis (volume of biodiesel per total volume of fuel). By definition, the molar and volumetric blends are related by:

$$BD_{mol} = \frac{MW_{BD} \rho_{BD}}{MW_{D} \rho_{D}}$$

where $MW_{vol}$ is the volumetric biodiesel blend fraction. The $MW$ and $\rho$ terms represent molecular weight and density, respectively.

Equations (5), (6), and (7) allow for the prediction of exhaust oxygen levels as a function of mixture fraction and volumetric biodiesel blend. Fig. 2 displays predicted exhaust $O_2$ mole fractions across mixture fractions from 0.015 to 0.050 (air-fuel ratios from 65 to 19) for B0, B20, B40, B60, B80, and B100 blends of soy-based methyl ester biodiesel. This range of mixture fractions is of the greatest interest for combustion in diesel engines. The numeric values of the parameters used are given in Table I.

![Fig. 2. Model Predictions: $O_2$ vs. Mixture Fraction for Soy-Based Methyl Ester Biodiesel Blends B0, B20, B40, B60, B80, & B100](image)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
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<tbody>
<tr>
<td>atomic mass of carbon</td>
<td>$a_C$</td>
<td>12.011</td>
<td>kg/kmol</td>
</tr>
<tr>
<td>atomic mass of hydrogen</td>
<td>$a_H$</td>
<td>1.0079</td>
<td>kg/kmol</td>
</tr>
<tr>
<td>atomic mass of oxygen</td>
<td>$a_O$</td>
<td>15.999</td>
<td>kg/kmol</td>
</tr>
<tr>
<td>atomic mass of nitrogen</td>
<td>$a_N$</td>
<td>14.007</td>
<td>kg/kmol</td>
</tr>
<tr>
<td>C atoms per diesel molecule</td>
<td>$n_C$</td>
<td>14.01$^a$</td>
<td>none</td>
</tr>
<tr>
<td>H atoms per diesel molecule</td>
<td>$m_H$</td>
<td>25$^a$</td>
<td>none</td>
</tr>
<tr>
<td>O atoms per diesel molecule</td>
<td>$r_O$</td>
<td>0$^a$</td>
<td>none</td>
</tr>
<tr>
<td>C atoms per biodiesel molecule</td>
<td>$n_{BD}$</td>
<td>18.82$^b$</td>
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</tr>
<tr>
<td>H atoms per biodiesel molecule</td>
<td>$m_{BD}$</td>
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<td>O atoms per biodiesel molecule</td>
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</tr>
<tr>
<td>mole ratio of $N_2$ to $O_2$ in air</td>
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</tr>
<tr>
<td>density of diesel</td>
<td>$\rho_D$</td>
<td>855.9$^a$</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>density of biodiesel</td>
<td>$\rho_{BD}$</td>
<td>879.6$^a$</td>
<td>kg/m$^3$</td>
</tr>
</tbody>
</table>

$^a$ As reported by Ref. [15]
$^b$ Calculated from soybean oil fatty acid profile reported by Ref. [1]
the distinction between blends becomes more substantial as the mixture fraction increases because a greater percentage of fuel is present in the fuel-air mixture (and the fuel is the cause for the distinction). This distinction in O₂ levels between different blends provides the basis for the estimation of the biodiesel blend given O₂ and mixture fraction. Interestingly, while (5) is clearly not exactly linear with respect to mixture fraction, the relationship between O₂ and mixture fraction shown in Fig. 2 appears to be nearly linear. It also appears that the slope of the lines is nearly linear with respect to the volumetric blend fraction (although it can be shown from (5), (6), and (7) that this is not exactly true). The implications of these two seemingly linear relationships will be discussed in detail later.

B. Direct Blend Estimation From O₂ & Mixture Fraction

The most direct method of estimating biodiesel blend levels given exhaust O₂ and mixture fraction is to combine (5), (6), and (7) and solve for BDvol. The result is (9) which explicitly gives the volumetric biodiesel blend fraction as a function of two known quantities, mixture fraction and exhaust O₂ mole fraction (all other parameters are constant).

\[
BD_{vol} = \left(1 - \frac{MW_{BD} \rho_{BD} (Nn_{BD} + Mm_{BD} + Rr_{BD})}{MW_{BD} \rho_{D} (Nn_{D} + Mm_{D} + Rr_{D})}\right)^{-1}
\]

\[
= function(x_{O_2}, f)
\]

where

\[
N = \left(\frac{1-f}{f}\right) x_{O_2} - 1,
\]

\[
M = \left(\frac{1-f}{f}\right) \beta - \left(\frac{1-f}{f}\right) \beta (\epsilon + 1) + \frac{1}{4} x_{O_2} - \frac{1}{4},
\]

\[
R = \left(\frac{1-f}{f}\right) \gamma - \left(\frac{1-f}{f}\right) \gamma (\epsilon + 1) + \frac{1}{2} x_{O_2} + \frac{1}{2}
\]

C. Simplified Blend Estimation From O₂ & Mixture Fraction

Fig. 2 indicates that O₂ levels are approximately linear with respect to mixture fraction, that is:

\[
x_{O_2} \approx a_1 f + b_1
\]

where \(b_1\) is constant and \(a_1\) is constant with respect to mixture fraction. Additionally, it appears that the slope, \(a_1\), of the lines in Fig. 2 is approximately linear with respect to the volumetric blend level, that is:

\[
a_1 \approx a_2 BD_{vol} + b_2
\]

where \(a_2\) and \(b_2\) are constants. Combining (9) and (10) yields (11), a simplified form of (9) which indicates that the volumetric blend level is approximately equal to a constant times \(x_{O_2}/f\), plus a constant times \(1/f\), plus a third constant.

\[
BD_{vol} \approx C_1 \left(\frac{x_{O_2}}{f}\right) + C_2 \left(\frac{1}{f}\right) + C_3
\]

where \(C_1 = a_2 / a_1\), \(C_2 = -b_1 / a_2\), and \(C_3 = -b_2 / a_2\). The values of \(C_1\), \(C_2\), and \(C_3\) which cause (11) to most closely reflect (9) can be found via the least squares best fit. Using the numeric values given in Table I, the best fit over the region where 0.015 \(\leq f \leq 0.050\) and 0 \(\leq BD_{vol} \leq 1\) is:

\[
BD_{vol,best,fit} = 2.415 \left(\frac{x_{O_2}}{f}\right) - 0.5064 \left(\frac{1}{f}\right) + 7.793
\]

Fig. 3 displays exhaust O₂ mole fractions as predicted by the direct method (Equations 5-7) as well as by the least squares best fit method (12). The fit is nearly perfect by visual inspection. In fact, the maximum difference between (9) and (12) across this region is than 0.0095 (less than the difference between B99 and B100). The coefficient of determination (R²) was also 0.9999. This strongly indicates that the complex equation (9) can be very accurately captured by a much simpler equation in the form of (11).

III. STEADY-STATE EXPERIMENTAL VALIDATION

A. Experimental Setup

The engine used was a 325-hp inline 6-cylinder 2007 Cummins 6.7 liter 24-valve ISB series engine with a variable geometry turbocharger (VGT), common rail fuel injection, and cooled EGR. Intake air flow was measured via a laminar flow element. Fuel flow was determined gravimetrically. The wideband oxygen sensor used was a commercial grade Bosch LSU 4.9 (Bosch #0258017025).

B. Experimental Procedure

Four fuels blends were tested: B0, B20, B50, and B100. The B0 fuel used was 2007 Emission Certification Ultra Low Sulfur Diesel Fuel. The B100 used was soy-based methyl ester biodiesel produced by Chevron Phillips. The B20 and B50 fuel blends were produced by mixing the B0 and B100 fuels on a volumetric basis. For each fuel blend, the engine was operated at 15 steady-state torque-speed points.
C. Experimental Results

Fig. 4 and Table II displays the experimental data collected for all four blends. The least squares best fit lines for all blend are also shown. While the slopes of the best fit lines are slightly steeper than what the model predicts (compare Fig. 4 with Fig. 2), the trends are the same. The coefficients of determination ($R^2$) for all blends exceed 0.99, supporting the assumption, (9), that $O_2$ is essentially linear with respect to mixture fraction. The B50 data also falls approximately halfway between the B0 and B100 data and the B20 data is slightly closer to B0 than B50. This supports the assumption, (10), that the slope of the lines is essentially linear with respect to the volumetric blend.

D. Performance of Estimator on Experimental Data

If (12), which is based purely on the theoretical model, is used to estimate the blend, it consistently underestimates the blend (although the trend is correct), as can be seen in Table III. The values shown are the mean estimated value for all 15 torque-speed points at each blend. A much more accurate estimator can be developed by “training” the estimator in the form of (11) with a portion of the experimental data. To do this, the odd numbered data points for B0 and B100 (16 data points total) were used to find “trained” values of $C_1$, $C_2$, and $C_3$ using the least squares best fit method. The resulting estimator is (13) which, when applied to all 60 data points, yields much more accurate results (within 4.2%), as can be seen in Table III.

\[ BD_{vol,best\ fit} = 2.158 \left( \frac{x_{O_2}}{f} \right) - 0.4665 \left( \frac{1}{f} \right) + 7.578 \] (13)

IV. CONCLUSIONS

Results from both the theoretical model as well as the experimental data presented in this work strongly indicate that exhaust oxygen content, as measured by a commercial grade wideband $O_2$ sensor, coupled with knowledge of the mixture fraction, can be used to estimate the biodiesel blend in a diesel engine operating at steady-state conditions. Furthermore, this estimation can be accomplished by an estimation algorithm with a very simple form:

\[ BD_{vol} \approx C_1 \left( \frac{x_{O_2}}{f} \right) + C_2 \left( \frac{1}{f} \right) + C_3 \]

where $BD_{vol}$ is the volumetric biodiesel blend fraction, $x_{O_2}$ is the exhaust $O_2$ mole fraction, $f$ is the mixture fraction, and $C_1$, $C_2$, and $C_3$ are constants.
Experimental results indicate that while the trained estimator algorithm works well at predicting the blend when applied to a number of data points, there is significant variation on a point by point basis (See Fig. 4). This seems unlikely to present an issue for practical implementation, however, because in an actual vehicle the fuel blend being delivered to the cylinders would take many minutes to change significantly, and the estimator algorithm could be implemented in a “continuously updating estimate” fashion.

“Narrow-band” O₂ sensors have been widely used with spark-ignited (SI) gasoline engines since the late 1970’s. Wideband O₂ sensors, which enable accurate measurements under highly lean (as well as rich) conditions have also been widely used with production SI gasoline engines for several years. Wideband O₂ sensors are now being used in a few diesel vehicles being produced today (such as the 2007 Dodge Ram with the 6.7 liter Cummins ISB engine). All this indicates that a wideband O₂ sensor is a very practical sensor that, when coupled with knowledge of the mixture fraction allows for the accurate estimation of biodiesel content in a fuel blend at steady-state. This estimation strategy is a major step towards achieving the goal of practical, real-time, on-board estimation and accommodation of alternative fuels in diesel engines.

V. FUTURE WORK

In future work a detailed error analysis will be pursued to quantify, in detail, the effect of inherent mixture fraction estimate error, exhaust oxygen measurement error, as well as variations in biodiesel feedstock and natural variations in the conventional diesel fuel. Future work will also focus on extending the estimator to account for dynamic engine operation, specifically the dynamics associated with the EGR system and the gas flow between the exhaust valves and the downstream location of the O₂ sensor.

It should also be noted that the estimation strategy presented in this work may have application outside biodiesel blends in diesel engines. The approach should theoretically be of use in any application where blends of two fuels with significantly different stoichiometric air-fuel ratios are being combusted in such a manner that the assumption of lean, complete combustion in idealized air to form major products is a reasonably good assumption. Examples include ethanol-diesel blends in diesel engines, ethanol-gasoline blends in lean-burn SI or HCCI/PCCI engines, as well as oxygenated fuel blends in non-automotive engines, such as gas turbine engines.

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