Dual-Fuel Solutions At Low Additive Percentages For Minimizing Pollutant Emission Formation And Maximizing Energy Generation

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Abstract—The goal of this research is to compile information on different dual-fuel solutions and to compare the pollutant formation and total heat release. The overall goal was to determine which dual-fuel solutions have the potential to maintain the desired power output while decreasing the production of NO_x and other pollutants in the exhaust. The overall carbon footprint created by the fuels was not considered. While natural gas as a base fuel produced the lowest overall pollutants, it also generated the lowest heat release when combusted. Alternatively, diesel as the base fuel had one of the highest energy outputs but had the greatest pollutant emission formation. Gasoline-Ethanol had the highest heat release per unit mass of pollutant (NO_x and OH) at higher temperatures. There were some outliers in the estimated pollutant formation which warrants further study.

Introduction and Background

The reliance on fossil fuels in the transportation sector have had a profound environmental impact with the production of pollutants such as CO₂, OH, and NO_x. These pollutants have had a major effect on the environment and on the health effects of people. This has spurned political action in many nations, creating new reforms regarding pollutant formation [1]. As a result, researchers have been working on finding ways to mitigate harmful pollutants during combustion [2]. This has been done by substituting typical combustion engines with other types of fuels and by utilizing mixtures of fuels to increase performance while minimizing pollutant emission formation.

Bio-fuels from agricultural products (oxygenated by nature) reduce the dependence on oil imports, support local agricultural industries and offer benefits in terms of usually reduced exhaust emissions. Among those fuels, bio-alcohols are considered as very promising. At the present time, bio-ethanol is the primary alternative to gasoline for spark-ignition engines, however bio-butanol has become a very competitive biomass-based renewable fuel. If compared with other alcohols, n-butanol has higher energy content and miscibility with gasoline, lower hygroscope and corrosive properties making it an attractive solution for gasoline replacement [2,3,4,5].

Mixtures of two different fuel sources are called dual-fuel solutions. These dual-fuel systems have shown potential to decrease pollutant emission and the depletion of non-renewable resources and some have already seen everyday use such as ethanol-gasoline mixtures in automobiles [2][7]. Recently, many researchers have been analyzing other types of dual-fuels to minimize harmful pollutants. The goal for many of these studies

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was to find a fuel source that decreases the production of many harmful pollutants [8]. Many of these solutions accomplish this by substituting non-renewable fuel sources by small amounts of other fuels such as alcohols and H_2 gas [9]. Other fuels use other types of fossil fuels and add small amounts of trace other compounds to burn all the fuel quickly [10]. The result of this versatility results in many combinations of dual-fuel solutions.

Despite these benefits, there are several concerns that get raised when using dual-fuel solutions for combustion processes. One of the biggest concerns with regards to dual-fuel solutions come from changes in the engine power output from burning these fuel combinations. By adding another fuel type to the fuel source, the combustion properties of the mixture changes. Some of these changes can affect the speed of the reaction, while others may have an impact on the heat release and power output [10]. How drastic this change is dependent on the percentages of each constituent present in the dual-fuel source [11].

Determining the usable energy output from these combustion processes can help determine the overall effectiveness of the dual-fuel solutions. Fuels that do not produce as much power compared to others requires more to be burned to generate the desired engine output. This has the opportunity to generate higher amounts of NO_x and other pollutants in the products. Thus, researchers must find ways of minimizing the pollutant emission, while maximizing the usable energy produced.

This has been a major field of study in combustion and automotive fields for the past few decades [12]. This has generated a large number of papers and experimental data on the performance and behavior of these dual-fuel solutions. Recent research has shown that butanol, instead of ethanol, has the potential of introducing a more suitable blend in diesel engines. This is because butanol has properties similar to current transportation fuels in comparison to ethanol. However, the main downside is the high cost of the butanol production process. Acetone-butanol-ethanol (ABE) is an intermediate product of the fermentation process of butanol production. By eliminating the separation and purification processes, using ABE directly in diesel blends has the potential of greatly decreasing the overall cost for fuel production. This could lead to a vast commercial use of ABE-diesel blends on the market [13]. The goal of this article is to compare the experimental data for several dual-fuel solutions and help consolidate information for other researchers in this field.

Methodology

To gain a proper understanding on the behavior of these different dual-fuel solutions, multiple sources for each mixture were considered. This provided data sources to compare manual calculations to and to generate a trend on what to expect in the results. This research helped to formulate predictions on how each mixture would behave, even at low percentages.

Determining the Dual-Fuel Sources Being Researched

The dual-fuel solutions researched were determined based off how common the fuels are in everyday society or those that have been commonly used in experiments within the past couple years. It is important to note that this is not a comprehensive list of all dual-fuel sources experimented on within the past few years, or a list of the most commonly researched fuels.

It is also important to understand that this article only focusses on the pollutant production and energy production of these dual-fuel solutions. Any other negative effects that could result from the combustion of these fuels will not be considered in the results. Some benefits and detriments of the fuels will be listed here and will not be used to draw any final conclusions.

Diesel-Methanol

Alcohols, like methanol, are a common additive in dual-fuel solutions. This is because alcohols are easy to produce from plant matter, and the presence of oxygen within the fuel itself results in lower amounts of air being needed for the combustion process to take place [12]. This is important in generating lower amounts of NO_x pollutants [8][14]. This creates a renewable aspect to the fuel helping to offset the use of the non-renewable diesel fuel.

Unfortunately, methanol does not mix well with diesel when water is present, and it can be difficult to sustain a mixture for very long [12]. This could be problematic during the combustion process. When the solution is properly mixed, the fuel should perform well.

Gasoline-Ethanol

Most commonly used in internal combustion engines found in automobiles and other equipment.[2][3] It is a mixture that is sold throughout the United States and other countries as a common fuel mixture in cars. Like methanol and other alcohols, ethanol is added to the fuel to help decrease the amount of air needed for the combustion reaction to occur. This is due to the present of oxygen in the compound which can help reduce the production of harmful pollutants such as NO_x gases.

Diesel-Hydrogen Gas

Hydrogen gas is highly reactive with oxygen, especially at high temperatures and pressures. Diesel, by comparison is fairly slow to combust [10]. This slow combustion rate can lead to high amounts of soot (unburned hydrocarbons) to be found in the exhaust. This is very problematic because it shows that fuel is being wasted and being released into the environment where it can pose health risks to individuals and animals. Some researchers hope to reduce soot emissions by injecting hydrogen gas into diesel engines.

Although hydrogen gas has the potential to decrease the amount of time needed for complete combustion to occur, it can also lead to other unwanted side effects of burning hydrogen gas or hydrogen in general [9]. The research performed in this article mainly focused on pollutant formation and heat release of the

compounds. The benefits and consequences of burning hydrogen gas in a dual-fuel solution warrants its own research.

Natural Gas-Hydrogen Gas

Natural gas is a popular base fuel for dual-fuel solution research. Although it is technically a fossil fuel, it contains less carbon and hydrogen in the molecule compared to other fuels such as gasoline and diesel fuels. This makes it a popular replacement for other, larger molecules in combustion processes.

Despite the benefit as a potential way to decrease the pollutant generation rate, it does have some problems for use in IC engines. The first issue is that it has a decrease power output which could result in more fuel needed to be burned for the desired power output. The second is that it has difficulty initiating and maintaining a combustion reaction in an IC engine due to its slow ignition speed [10]. As a result, it requires aid from an additional fuel to undergo a complete and stable reaction.

Hydrogen gas is known to burn quickly when used as an additive to other fuels [10]. Using it as an additive in this case should behave similarly to the diesel-hydrogen gas dual-fuel solution. Once hydrogen gas starts to burn, it will create a domino effect inside the engine, eventually leading to the combustion of the natural gas.

Natural Gas-Diesel

Natural Gas-Diesel is used by researchers similarly to natural gas-hydrogen gas. It is a fuel designed to get natural gas to combust in IC engine conditions while using an additional fuel to initiate the reaction. Diesel fuel specifically is chosen as an additive for natural gas to adapt it for use in an IC engine [15].

This is the only fuel in this study that is a mixture of two different fossil fuels. Since diesel is being added to generate the reaction, it would increase the amount of CO₂ in the products compared to a reaction of natural gas alone. Furthermore, this reaction (along with the natural gas-hydrogen gas reaction) is designed to lower pollutant emission by using a lower polluting base fuel compared to other fuels on this list. The additives for these mixtures are only used to start the reaction and are not designed to decrease pollutant formation. This could lead to a higher theoretical pollutant formation in the dual-fuel mixture compared to the base fuel being burned alone.

Formulating Data:

After gathering all of the necessary data, it was time to calculate the theoretical values. This was first done by choosing the specific fuels out of all those researched with enough data to get a proper comparison. Once these fuels were chosen, pollutant formation needed to be found. This was done with assistance from the software from Turns [16] called TPEQUIL[17]. This software assumes total combustion occurs. This means that the predictions made for pollutant formation will not include any of the original fuel in the products. Using the mole fractions of the products is found, one can find the total number of moles of each constituent. The software calculates the number of moles of fuel needed per mole of product. Using this value, an estimate of the total amount of products formed in kilomoles can be acquired.

$$N = \frac{x}{\frac{moles\ of\ reactant}{moles\ of\ product}}\tag{1}$$

This is important because the calculation is made for a single mole of fuel. Since the software gives the amount of fuel needed for a single mole of products, one can find the total number of products produced by a single mole of fuel by taking the inverse of that value. This is then multiplied by the mole fraction of the product to get the total number of moles formed.

After calculating the pollutant formation, the total energy released when burning the fuel can be derived. Using equation 2 (below), one can find the total heat release of the fuel at any temperature T compared to a reference temperature of 298.15 K.

$$q = \sum_{i=1}^{n} (\Delta h_i + h^o_{f,i} + \bar{R} T) x_i$$
 (2)

Where n is the total number of constituents in the reactants. Once this is found, one can divide the heat release by the number of moles of a specific product to find the amount of heat released per mole of fuel formed. This ratio will be used to compare the power potential of the fuel with the pollutant formation. This will give a lower value for a fuel with a large amount of pollutant formation while giving a higher value to fuels that do not produce as much.

This process will be repeated for each fuel for different percentages of the fuel additive (no additive, 1%, 5%, and 10%). These low percentages will show how drastic the changes in the fuel behavior will be compared to the base fluid. These were also tested for three different temperatures (2000 K, 2500K, 3000K) to compare the behaviors at different temperatures. These processes were taken at atmospheric pressure, and an A/F ratio of 0.9 (lean).

Using the Software:

When entering the fuel into the software under the set conditions, the number of carbon, hydrogen, and oxygen atoms had to be manually entered. These values were found by treating the combustion formulation for a single kmol of fuel. Using the chemical formula of the base fuel and additives, and the percentage of the additive in the fuel, the total number of each atom was found. The software then gave the mole fractions of each constituent in the products. The operating temperature, pressure, and the equivalence ratio can all be changed on the interface.

This process was repeated for each fuel, ratio of base fuel and additives, and for each temperature.

Assumptions:

Due to the nature of the calculations, soot emission and the formation of NO_2 in the products were not tested. This is a direct result of the software used to help calculate the amount of each constituent in the products. As a result, the formation of this pollutant will be assumed to be negligible, and that complete combustion is occurring.

It was also assumed that the fuels are evenly mixed and that they are able to combust properly without any difficulty. This was to ensure that each mixture is able to have a best-case pollutant formation calculation without considering fluid separation or the inability to normally undergo combustion in these conditions. As a result, the data will be measuring the performance under idealized conditions.

Natural gas was assumed to behave similarly to methane (CH_4) for the calculations. This is because natural gas is mainly composed of methane and the varying chemical makeup could make calculations difficult or inaccurate. For maintaining consistency among calculations, this assumption was deemed

necessary. Similarly, the chemical formulas for diesel and gasoline were taken to be $C_{10.8}H_{18.7}$ and $C_{8.26}H_{15.5}$ respectively. Like the methane/natural gas assumption, this was used specifically to reduce the complexity of the simulation and ensure consistent data.

Results

The total number of pollutants formed along with all necessary data are found in the appendix. The thermodynamic properties for each fuel source were found from tables in the appendices from Turns.

Diesel-Methanol:

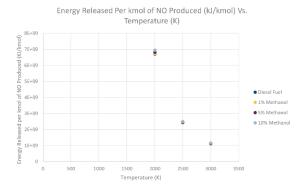


Figure 1: Energy release per kmol of NO produced for Diesel-Methanol (kJ/kg)

Table 1: NO formed at different temperatures for diesel-methanol

Percent	NO	NO	NO		
Methanol	Formation	Formation	Formation		
	at 2000 K	at 3000 K			
	(kmol)	(kmol)	(kmol)		
0	0.2063	0.7161	1.8542		
1	0.2044	0.7097	1.8376		
5	0.197	0.6839	1.771		
10	0.1877	0.6516	1.6879		

Table 2: OH formation at different temperatures for diesel-methanol

Percent	OH	OH	OH		
Methanol	Formation	Formation	Formation		
	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.1002	0.744	2.5688		
1	0.0994	0.7378	2.5475		
5	0.096	0.7128	2.462		
10	0.0918	0.6815	2.3552		

The diesel-methanol dual-fuel solution shows a decrease in NO production at as the percentage of the additive (methanol) increases for the same temperature. This is similarly shown for hydroxyl production. The total heat released by the combustion of the fuel per kmol of NO produced is higher for the 10% methanol reaction. This shows that there is a slightly higher energy gain for the 10% case for the same amount of pollutant formed compared to diesel being burned alone. This trend is less noticeable at higher temperatures.

Energy Released Per kmol of NO Formed Vs

Gasoline-Ethanol

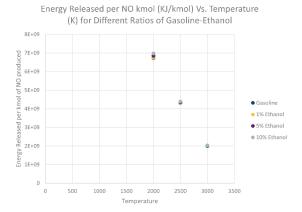


Figure 2: Energy release per kmol of NO produced for gasoline-ethanol (kJ/kg)

Table 3: NO formed at different temperatures for gasoline-ethanol

Percent	NO	NO	NO		
Ethanol	Formation	Formation	Formation		
	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.1617	0.5599	1.4485		
1	0.1605	0.5557	1.4377		
5	0.1556	0.5389	1.3946		
10	0.1495	0.5179	1.3406		

Table 4: OH formation at different temperatures for gasoline-ethanol

Percent	OH	OH	OH		
Ethanol	Formation	Formation	Formation		
	at 2000 K	at 2000 K at 2500 K			
	(kmol)	(kmol)	(kmol)		
0	0.0808	0.5997	2.075		
1	0.0803	0.5956	2.0611		
5	0.0781	0.5794	2.0058		
10	0.0753	0.5591	1.9366		

The NO and OH formation decrease with the addition of more ethanol in the fuel for reactions at the same temperatures. This trend is very similar to the diesel-methanol reaction; however, the pollutant formation is noticeably lower.

The energy release per kmol of pollutant shows that the 10% ethanol case yields more energy at all temperatures despite the difference being significantly lower at higher temperatures. This is an improvement over diesel-methanol which had all cases perform similarly at higher temperatures. This is possibly a result of the ethanol and gasoline molecules being closer in size to each other compared to diesel and methanol.

Diesel-Hydrogen Gas

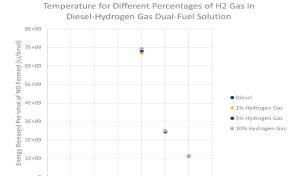


Figure 3: Energy release per kmol of NO produced for diesel-hydrogen gas (kJ/kg)

Table 5:NO formed at different temperatures for diesel-hydrogen gas

Temperature (K)

Percent	NO	NO	NO		
Hydrogen	Formation	Formation	Formation		
Gas	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.2063	0.7161	1.8542		
1	0.2049	0.7111	1.8409		
5	0.1963	0.6813	1.764		
10	0.1863	0.6465	1.6739		

Table 6: OH formation at different temperatures for diesel-hydrogen gas

Percent	OH	OH	OH		
Hydrogen	Formation	Formation	Formation		
Gas	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.1002	0.744	2.5688		
1	0.0999	0.7419	2.5262		
5	0.0955	0.7094	2.4497		
10	0.0909	0.6748	2.3305		

Diesel-Hydrogen gas behaves similarly to diesel-methanol. These two solutions have very similar pollutant formation rates with diesel-hydrogen gas producing similar or more pollutants at lower percentages of additive. This is possibly due to there only being a minute amount of additive in the fuel and to the larger size difference between hydrogen gas molecules with respect to diesel compared to methanol and diesel. At higher percentages of hydrogen gas in the fuel, the formation of NO and OH becomes lower than diesel-methanol. Much like the diesel-methanol combustion process, this fuel produces more energy per unit of NO produced at lower temperatures, and a negligible difference at higher temperatures.

Natural Gas-Hydrogen Gas

Energy Released Per kmol of NO Formed Vs. Temperature (K) For Different Percentages of Natural Gas-Hydrogen Gas Dual-Fuel Solution

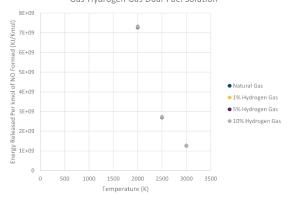


Figure 4: Energy release per kmol of NO produced for natural gashydrogen gas

Table 7: NO formed at different temperatures for natural gas-hydrogen gas

Percent	NO	NO	NO		
Hydrogen	Formation	Formation	Formation		
Gas	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.0266	0.0893	0.2297		
1	0.0264	0.0886	0.2279		
5	0.0256	0.0859	0.2208		
10	0.0246	0.0824	0.2119		

Table 8: OH formation at different temperatures for natural gashydrogen gas

Percent	ОН	OH	OH		
Hydrogen	Formation	Formation	Formation		
Gas	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.0168	0.1231	0.432		
1	0.0167	0.1713	0.4289		
5	0.0163	0.1192	0.4181		
10	0.0157	0.1153	0.4046		

Natural Gas-Hydrogen Gas showed a similar trend to the previous dual-fuel solutions researched. It had a visible decrease in the generation of pollutants such as NO and OH, with an outlier occurring at 1% hydrogen gas at 2500 K. While other dual-fuel solutions typically produce similar amounts of NO and OH during the combustion process, this fluid produces significantly more OH compared to NO at higher temperatures. This is heavily influenced by the presence of hydrogen gas in the fuel. Unlike the other solutions, this fuel has the smallest difference in energy release per kmol of NO produced. There is a barely noticeable difference at 2000 K and the difference gets harder to notice at higher temperatures.

Natural Gas-Diesel

Energy Released Per kmol of NO Formed Vs. Temperature (K) for Different Percentages of Diesel in the Natural Gas-Diesel Dual-Fuel Solution

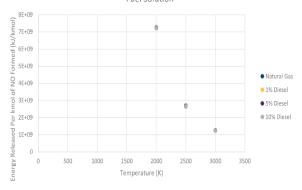


Figure 5: Energy release per kmol of NO produced for natural gas-diesel

Table 9: NO formed at different temperatures for natural gas-diesel

Percent	NO	NO	NO		
Diesel	Formation	Formation	Formation		
	at 2000 K	at 2000 K at 2500 K			
	(kmol)	(kmol)	(kmol)		
0	0.0266	0.0893	0.2297		
1	0.0106	0.0956	0.2459		
5	0.0143	0.1207	0.3108		
10	0.0189	0.152	0.3919		

Table 10: OH formation at different temperatures for natural gas-diesel

Percent	ОН	ОН	ОН		
Diesel	Formation	Formation	Formation		
	at 2000 K	at 2500 K	at 3000 K		
	(kmol)	(kmol)	(kmol)		
0	0.0168	0.1231	0.0432		
1	0.0176	0.1295	0.4289		
5	0.0211	0.1551	0.4181		
10	0.0253	0.1868	0.4046		

The natural gas-diesel dual fuel solution is the only dual-fuel solution to show an increase in pollutant formation compared to the base fluid at the same temperature. This is mainly seen in the formation of in the formation of OH at 2500 K and 3000 K.

Much like the natural gas-hydrogen gas, natural gas-diesel had a negligible difference between the energy release per NO formed for each percentage.

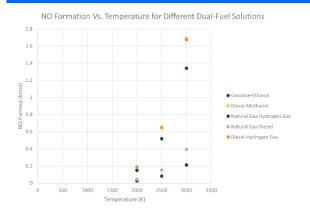


Figure 6: NO formation vs. temperature for different dual-fuel solutions

The NO formed during each combustion process is estimated using the above figure. At the same temperature, the natural gashydrogen gas produced the lowest amount of NO while fuels with diesel as the base produced the highest amount. Specifically, diesel-methanol produced the most NO compared to any other solution. Gasoline-ethanol only produced slightly less NO compared to the diesel-based fuels. Natural Gas-Diesel produced similar amounts of NO to natural gas-hydrogen gas. This difference increases with temperature.

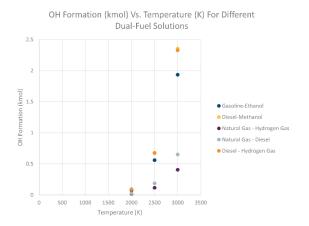


Figure 7: OH formation vs. temperature for different dual-fuel solutions

The formation OH experienced a similar trend to the production of NO. Natural Gas-Hydrogen Gas produced the lowest amount of OH followed closely by the natural gas-diesel fuel. Diesel based fuels performed poorly in comparison and produced similar levels of OH. Gasoline-Ethanol is not far behind the diesel-based fuels, producing slightly less OH at 2000 K. This difference increases as temperature increases.

Each of the dual-fuel solutions produce similar amounts of OH at 2000 K, but the values scatter apart as temperature increases.

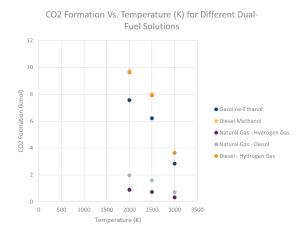


Figure 8: CO₂ formation vs. temperature for different dual-fuel solutions

The CO_2 formation decreased with respect to temperature for each solution. CO_2 formation decreases with temperature as a result of an increase in CO formation in the products. Despite this downward trend, diesel-based solutions still produced the most CO_2 . Natural gas based dual-fuel solutions produced the lowest amount of CO_2 for all temperatures due to the lower amounts of carbon in the fuel. Natural Gas-Hydrogen Gas is the lowest producer of CO_2 while natural gas-diesel produces slightly more.

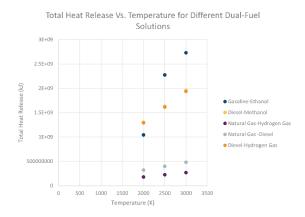


Figure 9: Total heat release vs. temperature for different dual-fuel solutions

The total energy release was highest for diesel-based dual-fuel solutions while at 2000 K, but gets surpassed by gasoline-ethanol at 2500 K and 3000 K. This means for higher operating temperatures, gasoline-ethanol produces more energy compared to diesel-methanol and diesel-hydrogen gas. The natural gas based dual-fuel solutions produced significantly less energy when burned compared to diesel and gasoline-based fuels. Gasoline-Ethanol is the only fuel on the list that did not have a linear increase in energy release with respect to temperature.

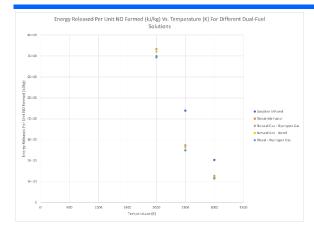


Figure 10: Energy release per unit NO formed (kJ/kg) vs. temperature (K) for different dual-fuel solutions

The energy release per kmol of NO formed was highest for natural gas-hydrogen gas at 2000 K but was replaced by gasoline-ethanol at higher temperatures. Diesel-Hydrogen Gas consistently had the lowest energy release per kmol of NO formed. These comparisons were made at 10% additive for all dual-fuel solutions.

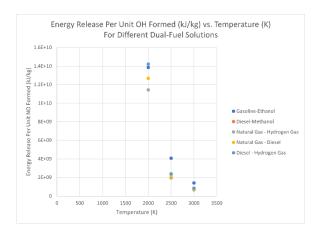


Figure 11: Energy release per unit OH formed vs. temperature for different dual-fuel solutions

Diesel-Hydrogen Gas held the highest energy release per kmol of OH produced at 2000 K while gasoline-ethanol had the highest heat release at higher temperatures. Natural Gas-Hydrogen Gas had the lowest heat release per kmol of OH produced for all temperatures.

Discussion

Most of the dual-fuel solutions decreased the formation of NO and OH pollutants at the same temperatures. The only dual-fuel solution that had a consistent increase in pollutant formation was natural gas-diesel. This increase is a direct result in diesel being used to initiate the combustion reaction instead of being used as a way to decrease pollutant formation. Despite this increase in pollutant formation, it had the second lowest pollutant formation compared to all of the dual-fuel solutions researched. Furthermore, it was able to produce the most energy per unit of NO formed at 2000 K. Despite this, it produced the second lowest amount of energy per kmol of OH produced.

Gasoline-Ethanol performed the best out of all the fuels at higher temperatures. It produced the most energy per unit of NO and OH formed. This is due to the high pollutant formation of dieselbased fuels and the low energy production of natural gas-based fuels. Gasoline-Ethanol under performs at 2000 K compared to the other fuels. Although it produced the second most energy per kmol of OH formed, it produced the second lowest amount of energy per kmol of NO.

Diesel-Hydrogen Gas produced the most amount of energy per kmol of OH formed. This fluid performed very similarly to Diesel-Methanol, partially because diesel fuel is a larger molecule compared to the additives. This size difference causes the diesel fuel properties to heavily influence the behavior of the fuel. This is why the performance of the two fuels were slightly shifted when compared to each other. As the percentages of the additive increase, and the additive is more pronounced in the fuel, the behavior of the two fuels will skew away from each other.

Similarly, the opposite is true for natural gas-based fuels. When the base molecule is small compared to the additives, the additives will have a greater effect on the fluid behavior. Since natural gas was assumed to be chemically similar to methane (CH₄), the additives were relatively larger compared to other fuels. Hydrogen gas, for example, has a significantly lower molecular weight compared to diesel and gasoline but comparing hydrogen gas with natural gas has a significantly lower difference in size. A larger fuel additive such as diesel in the natural gas fuel has a larger molecular weight by comparison and creates a significant shift in the behavior of the fluid compared to the hydrogen gas and original natural gas reactions. Natural Gas-Diesel was shown to almost double NO formation at 10% compared to the original natural gas reaction. This change is significant compared to changes shown when a fuel is added to diesel, especially with a small amount of diesel fuel added. Given the size of the diesel fuel relative to the natural gas, a small amount of diesel fuel is still a relatively large amount with respect to the natural gas. This change in behavior is shown to increase at higher temperatures.

At higher temperatures, the other dual-fuel solutions got similar results. Since NO and OH production is heavily related to temperature, the amount of pollutant formed increased significantly at higher temperatures for all fuels. This change in pollutant formation creates a non-linear growth, while energy release remains fairly linear for most fuels (excluding gasoline-ethanol). This shows that the change in pollutant formation increases faster compared to heat release, forming the decay trend in heat release per kmol of pollutant produced.

 ${\rm CO_2}$ formation would show a positive trend at higher temperatures compared to other pollutants due to CO molecules becoming more prevalent at higher temperatures. This negative trend in ${\rm CO_2}$ formation trades one pollutant for another and still creates adverse health and environmental effects and is not meant to be taken as a positive characterization of burning fuels at higher temperatures. Please refer to tables A.1.1-A.15.2 in the appendix for the complete breakdown of pollutant formation for the fuels at different temperatures for more information on ${\rm CO_2}$ and CO formation.

The pollutant formation found using these simulated calculations experienced similar trends to the researched data. There were some discrepancies between the values resulting from the assumptions and how the calculations were performed.

Errors

There are several major sources of error in the data.

As stated earlier, the software does not solve for all pollutants in the products. NO_2 , another oxide of nitrogen, is not calculated in the software. This is a major pollutant that is found in real world experimental data which has negative environmental and health effects. This also led to a higher amount of NO, N_2 , N, O, and O_2 in the estimate products compared to real world results. Solving for this will result in an increased accuracy in the theoretical solution.

Another major source of error compared to real life data stems from soot emissions. The reaction above was calculated under the assumption that complete combustion occurs. Decreasing soot emission leads to an increase in heat release and the production of other pollutants. Leaving unburned fuel in the products is very problematic and also creates environmental damage and can cause adverse health effects. Minimizing this can result in better combustion efficiency. Neglecting the amount of unburned fuel in the products will create a difference in pollutant data. Since dual-fuel solutions are often used to help minimize the soot emission in fuels, finding the amount of unburned fuel can help better understand what is happening during the combustion process.

Other errors stem from other assumptions made by this article. These include assuming that natural gas and methane behave similarly to each other. Other sources of error include a lack of separation during the combustion process, the fuel being perfectly mixed, and the use of methanol and ethanol with no water present in the mixture. These assumptions effect the combustion behavior and molecular interactions during the reaction. Under these idealized conditions, it is assumed the molecular interactions are evenly distributed. In real world conditions, fuel injection, when the fuel is injected, and the fluid properties all have an effect on the behavior of the combustion reaction. These fuels also undergo combustion under different conditions and result in requiring different set ups and hardware. Assuming an idealized combustion set up provides insight on how the combustion process will behave when it occurs in the proper set up. This, however, can cause discrepancies and errors with a real-world combustion process.

Summary and Conclusions

The goal of this article was to create a small compendium on the basics of dual-fuel reactions and show how they behave at low additive percentages. This involved researching multiple dual-fuel solutions and creating pollutant formation estimates. The research was used to gather background information and to provide a comparison with the theoretical calculations.

Researched behavior of the fuels determined that

The data showed that most of the dual-fuel solutions studied had reduced pollutant formation in the products. The only fuel that increased pollutant formation as additive increased was natural gas-diesel. Despite this trend, it had the highest heat release per kmol of NO formed at 2000 K. At higher temperatures, gasoline-ethanol outperformed the other dual-fuel solutions. At lower temperatures, diesel-hydrogen gas produced the highest amount of energy per kmol of OH formed.

The diesel-based fuels performed very similarly to each other, while the natural gas-based fuels had a larger difference in pollutant formation. This is due to the molecule size for diesel being significantly larger compared to the additives.

Although people are moving away from the use of fossil fuels in the automotive sector, dual-fuel solutions have the possibility of reducing the pollutant formation during this transition. Dual-fuel solutions are a temporary solution to minimizing certain pollution formation and will not solve the crisis between climate and energy. Although many dual-fuel solutions substitute the base fossil fuel with an additive containing an alcohol or enriched using a commonly found fuel such as hydrogen gas, they still are mainly fossil fuels. Finding ways to reduce the dependence on fossil fuels by making a mixture is a temporary solution until a more permanent solution is reached.

Recommendation:

Given the research and conclusions made by this research, the following recommendations for further research are proposed.

Research the performance of more dual-fuel solutions and compare them to each other and the previously researched fuels. These above fuels are common, but there are plenty of other dual-fuel solutions being researched using different base fuels and additives. These fuels possess different properties and finding ways to reduce the formation of pollutants.

Testing of these dual-fuel solutions at more temperatures can provide a deeper insight on the behavior of the fuels themselves. This can help find the operating temperature where gasoline-ethanol overtakes the other fuels as the fuel with the highest energy releaser per kmol of pollutant formed. It can also verify the trends shown in the data and determine if outliers in the data are truly outliers and not a result of some unidentified process.

Using the data from this research, a report on the total effect of the fuels can be researched. This involves going further into the pros and cons of each fuel. Although this article goes into the pollutant formation of the fuels under the same operating conditions, this is far from everything that occurs when fuel is being combusted. Some fuels and additives cause further changes in the combustion process and were not fully covered in this article. One example would be finding the percentage of additive needed to combust natural gas without having much difficulty. Another area of research that was discussed but not calculated for would be the amount of time needed for complete combustion to occur. Some fuels and additives, such as hydrogen gas, can have an impact on the reaction speed. The total impact this has on the combustion behavior was not fully investigated here and needs to be investigated further.

The total heat release calculated was based off combusting the reactants without calculating the formation of the products. This is not usable energy, but the total energy produced. This was used to make an estimate regarding the energy released by the reaction with respect to the formation of a particular pollutant. This was also used to discretize the data for a proper comparison. This does not give the total amount of usable energy generated from the reaction. The calculation for usable energy for each fuel at different temperatures and percentages should be considered in future articles. This will provide a greater picture on what is occurring and how much energy is used to create the pollutants. This will affect the best performing dual-fuel solutions depending on how much energy is consumed making the products.

Most dual-fuel solutions are designed with reducing pollutant formation and overall environmental impact without sacrificing performance. Although pollutant formation has a large impact on the environment, the production and transportation of the fuels adds to the overall carbon footprint of the fuel. This overall environmental impact of the fuel involves a deeper level of research and calculations that could provide an insight on whether a fuel is better for the environment. A fuel that produces less pollutants like NO_x and CO_2 is important to the future of energy, but if the fuel requires high levels of refinement, transport, or takes a large amount of energy to acquire, it may not be viable or ideal for reducing global pollutants production.

Nomenclature:

- N- Number of moles
- x- Mole fraction
- q Heat release
- Δh- Sensible Enthalpy
- hof- Enthalpy of formation
- \bar{R} Ideal gas constant
- T-Temperature

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There are no conflicts of interest regarding the information in this report.

Appendix:

T = 2500K				Moles of Fuel per Mole of Product								
1 – 2300K			Air	Froduct								
Methanol	Diesel	MW	(kmo									
(kmol)	(kmol)	fuel	1)	CO2	H2O	N2	Н	О	N	H2	OH	CO
			81.84						2.2018			
0	1	148.6	6	8.7969	8.58927	64.2930	0.13426	0.20473	E-05	0.32161	0.744	2.00308
		147.4	81.36						2.1822			
0.01	0.99	344	7	8.7170	8.52195	63.7124	0.13314	0.2029	E-05	0.3191	0.73775	1.98497
		142.7	79.45						2.1037			
0.05	0.95	72	2	8.3974	8.25272	61.39	0.12865	0.19565	E-05	0.30908	0.71277	1.91256
		136.9	77.05						2.0057			
0.1	0.9	44	9	7.998	7.91617	58.4869	0.12304	0.18641	E-05	0.29654	0.68153	1.82204

Table A.1.1: Diesel-Methanol at 2000 K

Methanol (kmol)				h for	h nitrogen	h oxygen	Moles of	Moles of	Heat	Per unit of NO Formed	Per Unit of OH Formed
(',	NO	O2	h for diesel	Methanol	gas	gas	O2	N2	Release KJ	(KJ/kmol)	(kJ/kmol)
0	0.71613	2.26892	1112667.175	42499.63087	74305	78346	17.19444	64.65111	1729312113	2414802137	2324351502
0.01	0.70967	2.24851	1112667.175	42499.63087	74305	78346	17.09389	64.27302	1719316216	2422681309	2330480467
0.05	0.68386	2.16688	1112667.175	42499.63087	74305	78346	16.69167	62.76067	1679332629	2455675000	2356065446
0.1	0.65159	2.06483	1112667.175	42499.63087	74305	78346	16.18889	60.87022	1629353145	2500595201	2390711341

Table A.1.2: Diesel-Methanol at 2000 K

T = 2500 K				Moles of Fuel per Mole of Products								
Methanol (kmol)	Diesel (kmol)	MW fuel	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	ОН	CO
0	1	148.6	81.8456	8.79692	8.58927	64.29304	0.13426	0.20473	2.2018 E-05	0.32161	0.744	2.0031
0.01	.99	147.43 44	81.3669	8.71702	8.521955	63.71241	0.13314	0.2029	2.1822 E-05	0.3191	0.73775	1.985
0.05	.95	142.77 2	79.4523	8.39745	8.25272	61.38997	0.12865	0.19565	2.1037 E-05	0.30908	0.71277	1.91256
0.1	0.9	136.94 4	77.0591	7.99797	7.91617	58.48687	0.12304	0.18641	2.0057 E-05	0.296545	0.68153	1.822

Table A.2.1 Diesel-Methanol at 2500 K

Methanol	NO	O2	h for diesel	h for	h	h	Moles of	Moles of	Heat	Per unit of	Per Unit of
(kmol)				Methanol	nitrogen	oxygen	O2	N2	Release KJ	NO Formed	OH Formed
					gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.71613	2.26892	1112667.175	42499.63087	74305	78346	17.19444	64.65111	1729312113	2414802137	2324351502
0.01	0.70967	2.24851	1112667.175	42499.63087	74305	78346	17.09389	64.27302	1719316216	2422681309	2330480467
0.05	0.68386	2.16688	1112667.175	42499.63087	74305	78346	16.69167	62.76067	1679332629	2455675000	2356065446
0.1	0.65159	2.06484	1112667.175	42499.63087	74305	78346	16.18889	60.87022	1629353145	2500595201	2390711341

Table A.2.2 Diesel-Methanol at 3000 K

T=				Moles of								
3000				Fuel per								
K				Mole of								
				Product								
Metha	Diesel	MW	Air	CO2	H2O	N2	Н	O	N	H2	OH	CO
nol	(kmol)	fuel	(kmol)									
(kmol)	()		()									
()												
0	1	148.6	81.8455	4.03463	5.82048	63,72345	1.78329	2.08214	0.00108	1.35346	2.56883	6.76537
-			6									
0.01	0.99	147.4	81.3669	3.998	5.77551	63.14795	1.76848	2.06361	0.00107	1.34302	2.54747	6.704
		344	1									
0.05	0.95	142.7	79.4523	3.85147	5.59563	60.84583	1.70923	1.98946	0.00103	1.30124	2.462022	6.45908
		72	3									
0.1	0.9	136.9	77.0591	3.6683	5.37081	57.96823	1.63515	1.89677	0.0001	1.24902	2.3552	6.1517
	1	44	1 1									

Table A.3.1 Diesel-Methanol at 3000 K

Methanol	NO	O2	h for diesel	h for	h	h	Moles of	Moles of	Heat	Per unit of	Per Unit of
(kmol)				Methanol	nitrogen	oxygen	O2	N2	Release KJ	NO Formed	OH Formed
					gas	gas				(KJ/kmol)	(kJ/kmol)
0	1.85422	3.61429	1652274.501	171395.3076	92730	98036	17.19444	64.65111	2075791162	1119495722	808069999.4
0.01	1.83759	3.58208	1652274.501	171395.3076	92730	98036	17.09389	64.27302	2063792367	1123100306	810134928.1
0.05	1.77104	3.45324	1652274.501	171395.3076	92730	98036	16.69167	62.76067	2015797188	1138198251	818756893.8
0.1	1.68787	3.29219	1652274.501	171395.3076	92730	98036	16.18889	60.87022	1955803214	1158743731	830420315.8

Table A.3.2 Diesel-Methanol at 3000 K

T =				Moles of								
2000				Fuel per								
K				Mole of								
				Product								
Ethano	Gasolin	MW	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	OH	CO
1	e	fuel										
(kmol)	(kmol)											
0	1	114.8	64.1806666	8.18187441	7.69250604	50.6164703	0.00171613	0.00626772	0	0.01621842	0.08083254	0.07812379
			7	8	8	6	1	6		2	5	7
0.01	0.99	114.112	63.9156933	8.11985998	7.64538371	50.2354352	0.00170482	0.00622082	0	0.01611978	0.08028378	0.07753820
		7	3	9	1	6	7	8		3	2	5
0.05	0.95	111.363	62.8558	7.87180641	7.45689884	48.7113247	0.00165810	0.00603399	0	0.01572737	0.07808830	0.07519335
		5		3	3	7	3	8			7	2
0.1	0.9	107.927	61.5309333	7.56173822	7.22129186	46.8061751	0.00160093	0.00580047	0	0.01523759	0.07534301	0.07226293
			3	3	7	8	5	1		4	5	4

Table A.4.1 Gasoline-Ethanol at 2000 K

	NO	O2	h for Gas	h for ethanol	h	h	kmoles of	kmoles of	Heat	Per unit of	Per Unit of
					nitroge	oxyge	O2	N2	Release KJ	NO Formed	OH Formed
					n gas	n gas				(KJ/kmol)	(kJ/kmol)
Ethano	0.16170869	1.29173675	662906.335	6047.27466	56130	59169	13.4833333	50.6973333	108819564	672935784	1346234554
1	1	3	3	7			3	3	9	5	7
(kmol)											
0	0.16049114	1.28201133	662906.335	6047.27466	56130	59169	13.4276666	50.4880266	108376779	675281980	1349921208
	7	1	3	7			7	7	7	1	3
0.01	0.15562150	1.24310857	662906.335	6047.27466	56130	59169	13.205	49.6508	106605638	685031530	1365193374
	6	2	3	7					8	9	0
0.05	0.14953439	1.19448046	662906.335	6047.27466	56130	59169	12.9266666	48.6042666	104391712	698111731	1385552636
	1	6	3	7			7	7	6	2	7
0.1	0.14953439	1.19448046	662906.335	6047.27466			12.9266666	48.6042666	104391712	698111731	1385552636
	1	6	3	7	56130	59169	7	7	6	2	7

Table A.4.2 Gasoline-Ethanol at 2000 K

T= 2500 K				Moles of Fuel per Mole of								
				Product								
Ethan	Gasolin	MW	Air (kmol)	CO2	H2O	N2	H	O	N	H2	OH	CO
ol	e	fuel										
(kmol)	(kmol)											
0	1	114.8	64.180666	6.7223395	7.1276967	50.417393	0.1087119	0.1602953	1.73175	0.2680970	0.5997008	1.5376673
			67	58	74	6	01	13	E-05	03	91	83
0.01	0.99	114.112	63.915693	6.6713198	7.0842118	50.409465	0.1079827	0.1591047	1.71899	0.2664754	0.5956451	1.5260811
		7	33	53	51	63	06	24	E-05	69	84	75
0.05	0.95	111.363	62.8558	6.4672660	6.9102690	48.519707	0.1050644	0.1543436	1.66792	0.2599911	0.5794178	1.4797360
		5		07	69	51	82	06	E-05	93	28	68
0.1	0.9	107.927	61.530933	6.2121955	6.6928403	46.621988	0.1014157	0.1483925	1.60409	0.2518865	0.5591277	1.4218021
			33	84		24	71	4	E-05	72	59	64

Table A.5.1 Gasoline-Ethanol at 2500 K

Ethanol	NO	O2	h for Gas	h for ethanol	h	h	kmols of O2	kmols of N2	Heat	Per unit of	Per Unit of
(kmol)					nitrogen	oxygen			Release KJ	NO Formed	OH Formed
					gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.559859465	1.768390362	1237991.635	80906.18233	74305	78346	24.11764706	90.68235294	2416913415	4317000189	4030198136
0.01	0.555658771	1.755164528	1237991.635	80906.18233	74305	78346	23.9732563	90.1394437	2402563801	4323811529	4033548603
0.05	0.538855271	1.479736068	1237991.635	80906.18233	74305	78346	23.39569328	87.96780672	2345165346	4352124721	4047451135
0.1	0.517850005	1.636127981	1237991.635	80906.18233	74305	78346	22.6737395	85.2532605	2273417277	4390107670	4066006809

Table A.5.2 Gasoline-Ethanol at 2500 K

T =				Moles of	0.0135804	0.0136810	0.0140989	0.0146586				
3000				Fuel per	0.0133004	6	0.0140707	0.0140300				
K				Mole of	3	U	4	2				
K												
				Products								
Ethan	Gasoli	MW	Air (kmol)	CO2	H2O	N2	H	О	N	H2	OH	CO
ol	ne	fuel										
(kmol	(kmol)											
)												
0	1	114.8	64.180666	3.0752516	4.8535952	49.972650	1.4482943	1.6291317	0.0008468	1.1347770	2.0749608	5.1847474
			67	67	1	35	47	73	07	28	08	64
0.01	0.99	114.112	63.915693	3.0519294	4.8246042	49.596401	1.4386480	1.6171356	0.0008405	1.1280076	2.0611239	5.1454682
		7	33	56	34	89	29	61	78	25	19	61
0.05	0.95	111.363	62.8558	2.9586429	4.7086511	48.074808	1.4000570	1.5691534	0.0008149	1.1009338	2.0057692	4.9883551
		5		9	47	04	26	26	55	29	28	53
0.1	0.9	107.927	61.530933	2.8420356	4.5637242	46.210230	1.3518025	1.5091754	0.0007838	1.0670949	1.9365540	4.7919619
			33	08	8	57	57	89	39	93	55	99

Table A.6.1 Gasoline-Ethanol at 3000 K

Ethanol	NO	O2	h for Gas	h for	h	h	kmoles of	kmoles of	Heat	Per unit of	Per Unit of
(kmol)				ethanol	nitrogen	oxygen	O2	N2	Release KJ	NO Formed	OH Formed
					gas	gas				(KJ/kmol)	(kJ/kmol)
0	1.44850789	2.812609026	2305019.992	134961.196	92730	98036	24.11764706	90.68235294	2901535692	2003120392	1398356866
0.01	1.437716083	2.791875776	2305019.992	134961.196	92730	98036	23.9732563	90.1394437	2884305825	2006172052	1399384966
0.05	1.394550229	2.708947623	2305019.992	134961.196	92730	98036	23.39569328	87.96780672	2815386354	2018849014	1403644205
0.1	1.340593453	2.605289584	2305019.992	134961.196	92730	98036	22.6737395	85.2532605	2729237016	2035842418	1409326535

Table A.6.2 Gasoline-Ethanol at 3000 K

T = 2000 K				Moles of Fuel per Mole of Products								
Hydroge n Gas (kmol)	Diese 1 (kmol	MW fuel	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	ОН	СО
0	1	148.6	81.8455555 6	10.6980499 3	9.27931663 2	64.5479843 2	0.00212285 9	0.00798389	0	0.0195258	0.10019704 2	0.10195353 3
0.01	0.99	147.1341 6	81.3008	10.5910353	9.28942163 4	64.1183174	0.00211822 1	0.00793149 4	0	0.01955287 5	0.09992563 4	0.10096021 4
0.05	0.95	141.2708	79.1217777 8	10.1631338 9	8.86506262 9	61.4248603 9	0.00202469 5	0.00759755 4	0	0.01865671	0.0955399	0.09686881 2
0.1	0.9	133.9416	76.398	9.62821769 1	8.45080856 1	58.3017346 8	0.00192611 4	0.00721216 7	0	0.01778740 3	0.09088269 4	0.09178353

Table A.7.1 Diesel-Hydrogen Gas at 2000 K

Hydrogen	NO	O2	h for diesel	h for	h	h	Moles of O2	Moles of N2	Heat	Per unit of	Per Unit of
Gas				hydrogen	nitrogen	oxygen			Release KJ	NO Formed	OH Formed
(kmol)				gas	gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.206294957	1.648526947	717902.5747	52968	56130	59169	17.19444444	64.65111111	1383002891	6704007266	13802831505
0.01	0.204911415	1.637382254	717902.5747	52968	56130	59169	17.08	64.2208	1373906576	6704880621	13749290538
0.05	0.196308888	1.568681359	717902.5747	52968	56130	59169	16.62222222	62.49955556	1337521319	6813350797	13999609854
0.1	0.186322006	1.488835425	717902.5747	52968	56130	59169	16.05	60.348	1292039747	6934445227	14216565208

Table A.7.2 Diesel-Hydrogen Gas at 2000 K

T = 2500 K				Moles of Fuel per Mole of Products								
Hydrogen Gas (kmol)	Diesel (kmol)	MW fuel	Air (kmol)	CO2	Н2О	N2	Н	О	N	H2	ОН	СО
0	1	148.6	81.8455556	8.796921004	8.589267549	64.29303835	0.134257795	0.204732107	2.2018E- 05	0.321605376	0.743997675	2.003079877
0.01	0.99	147.13416	81.3008	8.707947655	8.599867317	63.8652431	0.133961329	0.203327131	2.18804E- 05	0.322202637	0.741896382	1.984050076
0.05	0.95	141.2708	79.12177778	8.356588036	8.206417027	61.18230896	0.128050498	0.194806022	2.0957E- 05	0.307366797	0.709377829	1.90341012
0.1	0.9	133.9416	76.398	7.916257871	7.823568923	58.07158569	0.121842908	0.184878905	1.9896E- 05	0.293128888	0.674755837	1.803739009

Table A.8.1 Diesel-Hydrogen Gas at 2500 K

Hydrogen	NO	O2	h for diesel	h for	h	h	Moles of O2	Moles of N2	Heat	Per unit of	Per Unit of
Gas				hydrogen	nitrogen	oxygen			Release KJ	NO Formed	OH Formed
(kmol)				gas	gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.716129941	2.268920722	1112667.175	70492	74305	78346	17.19444444	64.65111111	1729312113	2414802137	2324351502
0.01	0.711067798	2.251944728	1112667.175	70492	74305	78346	17.08	64.2208	1717937326	2415996521	2315602783
0.05	0.681337391	2.158234416	1112667.175	70492	74305	78346	16.62222222	62.49955556	1672438176	2454640240	2357612695
0.1	0.646544946	2.04754818	1112667.175	70492	74305	78346	16.05	60.348	1615564239	2498765552	2394294574

Table A.8.2 Diesel-Hydrogen Gas at 2500 K

T =				Moles of	0.0106836	0.0107504	0.0112243	0.0118227				
3000 K				Fuel per	2	7	3					
				Mole of								
				Products								
Hydrog	Diese	MW fuel	Air (kmol)	CO2	H2O	N2	Н	О	N	H2	OH	CO
en Gas	1											
(kmol)	(kmo											
	1)											
0	1	148.6	81.845555	4.0346315	5.8204775	63.723445	1.7832906	2.0821435	0.0010782	1.3534616	2.5688259	6.7653660
			56	2	16	8	82	06	86	54	22	46
0.01	0.99	147.134	81.3008	3.9924273	5.8316975	63.299823	1.7801119	2.0676584	0.0010715	1.3570792	2.5623316	6.6995759
		16		08	91	17	39	37	81	72	93	26
0.05	0.95	141.270	79.121777	3.8320006	5.5629903	60.640470	1.7012080	1.9810973	0.0010263	1.2940727	2.4496669	6.4280006
		8	78	63	97	3	01	13	42	87	29	02
0.1	0.9	133.941	76.398	3.6293714	5.3055029	57.557449	1.6191183	1.8800502	0.0009743	1.2346875	2.3304938	6.0906256
		6		63	73	65	06	42	97	08	8	61

Table A.9.1 Diesel-Hydrogen Gas at 3000 K

Hydrogen	NO	O2	h for diesel	h for	h	h	Moles of O2	Moles of N2	Heat	Per unit of	Per Unit of
Gas	110	02	ii ioi diesei	hydrogen	nitrogen	oxygen	Moles of O2	Moles of 142	Release KJ	NO Formed	OH Formed
(kmol)				gas	gas	gas			release 123	(KJ/kmol)	(kJ/kmol)
0	1.854219824	3.614292721	1652274.501	88733	92730	98036	17.19444444	64.65111111	2075791162	1119495722	808069999.4
0.01	1.840922304	3.586480405	1652274.501	88733	92730	98036	17.08	64.2208	2062136294	1120164762	804788973.6
0.05	1.764042932	3.437602066	1652274.501	88733	92730	98036	16.62222222	62.49955556	2007516821	1138020388	819506030.7
0.1	1.673863838	3.26091079	1652274.501	88733	92730	98036	16.05	60.348	1939242481	1158542551	832116530.1

Table A.9.2 Diesel-Hydrogen Gas at 3000 K

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				2.5.4								
T = 2000				Moles of								
K				Fuel per								
				Mole of								
				Products								
Hydroge	Natura	MW	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	OH	CO
n Gas	1 Gas	fuel	` ′									
(kmol)	(kmol)											
0	1	19	10.5672	0.99035595	1.40766964	8.34227994	0.00036333	0.00104550	0	0.00427266	0.01677948	0.00964404
				8		5	8	9		8	9	2
0.01	0.99	18.8301	10.4984444	0.98045110	1.97722996	8.27971359	0.00036103	0.00103777	0	0.0042519	0.01667532	0.00954882
		6	4	9	9	6	6	8			6	6
0.05	0.95	18.1508	10.1811111	0.94083187	1.93752581	8.02944653	0.00035222	0.00100676	0	0.00416920	0.01625836	0.94083187
			1	1	1	5	6			5	8	1
0.1	0.9	17.3016	9.78444444	0.89130801	1.88789588	7.71661256	0.00034117	0.00096795	0	0.00406512	0.01573667	0.00869203
			4	1	6			4		9	3	2

Table A.10.1 Natural Gas-Hydrogen Gas at 2000 K

Hydrogen	NO	O2	h for natural	h for	h	h	Moles of O2	Moles of N2	Heat Release	Per unit of	Per Unit of
Gas			gas	hydrogen	nitrogen	oxygen			KJ	NO Formed	OH Formed
(kmol)				gas	gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.026550323	0.211278611	48644.11145	52968	56130	59169	2.22	8.3472	192999496.4	7269195849	11502108255
0.01	0.026350596	0.209683231	48644.11145	52968	56130	59169	2.20555556	8.292888889	191852300.4	7280757523	11505160178
0.05	0.025551272	0.203301794	48644.11145	52968	56130	59169	2.138888889	8.042222222	186557522.8	7301300690	11474554351
0.1	0.024552278	0.195325086	48644.11145	52968	56130	59169	2.05555556	7.728888889	179939050.9	7328812826	11434377249

Table A.10.2 Natural Gas-Hydrogen Gas at 2000 K

T = 2500 K				Moles of Fuel per Mole of Products								
Hydrog	Natur	MW	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	OH	CO
en Gas	al Gas	fuel										
(kmol)	(kmol											
)											
0	1	19	10.5672	0.8064554	1.8536028	8.3108972	0.0234099	0.0259646	2.94311	0.0731503	0.1230834	0.1935443
				86	01	27	62	98	E-06	91	18	96
0.01	0.99	18.8301	10.498444	0.7983385	1.8443987	8.2485759	0.0232703	0.0257666	2.92165	0.0728119	0.1712892	0.1916613
		6	44	63	08	88	49	06	E-06	3	61	34
0.05	0.95	18.1508	10.181111	0.7658735	1.8075822	7.9992904	0.0227119	0.0249743	2.83581	0.0714590	0.1192054	0.1841264
			11	14	22	81	77	84	E-06	44	11	46
0.1	0.9	17.3016	9.7844444	0.7252982	1.7615610	7.6876837	0.0220135	0.0239839	2.7285E	0.0697715	0.1153211	0.1747017
			44	83	8	85	68	84	-06	51	92	28

Table A.11.1 Natural Gas-Hydrogen Gas at 2500 K

Hydrogen	NO	O2	h for natural	h for	h	h	Moles of O2	Moles of N2	Heat Release	Per unit of	Per Unit of
Gas			gas	hydrogen	nitrogen	oxygen			KJ	NO Formed	OH Formed
(kmol)				gas	gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.089313123	0.273012348	96962.12404	70492	74305	78346	2.22	8.3472	241329839.9	2702064733	1960701483
0.01	0.088622609	0.270838135	96962.12404	70492	74305	78346	2.20555556	8.292888889	239895237.8	2706930453	1400527021
0.05	0.085860406	0.262140855	96962.12404	70492	74305	78346	2.138888889	8.042222222	233274160.2	2716900271	1956909148
0.1	0.082407688	0.251269546	96962.12404	70492	74305	78346	2.05555556	7.728888889	224997813.1	2730301230	1951053475

Table A.11.2 Natural Gas-Hydrogen Gas at 2500 K

T = 3000 K				Moles of Fuel per Mole of Products								
Hydrogen	Natural	MW fuel	Air (kmol)	CO2	H2O	N2	H	О	N	H2	OH	CO
Gas	Gas											
(kmol)	(kmol)											
0	1	19	10.5672	0.359540532	1.303145373	8.240626685	0.318289208	0.262520644	0.000141918	0.321911623	0.432031956	0.640459468
0.01	0.99	18.83016	10.49844444	0.355860158	1.296859073	8.178852051	0.316421475	0.260511759	0.000140884	0.32047825	0.428904011	0.634139909
0.05	0.95	18.1508	10.18111111	0.341143111	1.271712942	7.931752266	0.308946985	0.252476857	0.00013663	0.314751527	0.418124175	0.608856937
0.1	0.9	17.3016	9.78444444	0.322758549	1.240278902	7.622876904	0.299595857	0.242433528	0.000131351	0.307609098	0.404628052	0.577241521

Table A.12.1 Natural Gas-Hydrogen Gas at 3000 K

Hydrogen	NO	O2	h for	h for	h	h	Moles of O2	Moles of N2	Heat Release	Per unit of	Per Unit of
Gas			natural gas	hydrogen	nitrogen	oxygen			KJ	NO Formed	OH Formed
(kmol)				gas	gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.229715311	0.428962795	148214.797	88733	92730	98036	2.22	8.3472	289666343.8	1260979701	670474347.3
0.01	0.22793385	0.425521664	148214.797	88733	92730	98036	2.20555556	8.292888889	287944292.4	1263280081	671349031.3
0.05	0.220803452	0.411758737	148214.797	88733	92730	98036	2.138888889	8.042222222	279996729.1	1268081301	669649702.4
0.1	0.211892614	0.394559802	148214.797	88733	92730	98036	2.05555556	7.728888889	270062274.9	1274524252	667433396.9

Table A.12.2 Natural Gas-Hydrogen Gas at 3000 K

T =				Moles of	0.08628332	0.08103756	0.06518534	0.05237795				
2000				Fuel per	0.00020352	0.00103750	0.0021022.	0.00207770				
K				Mole of								
				Product								
Diesel	Natura	MW fuel	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	OH	CO
(kmol	1 Gas											
)	(kmol)											
0	1	16.043	10.5777777	0.99035595	1.40766964	8.34227994	0.00036333	0.00104550	0	0.00427266	0.01677948	0.00964404
			8	8		5	8	9		8	9	2
0.01	0.99	17.3685	11.3433444	1.08742686	2.06006548	8.90433695	0.00038142	0.00111491	0	0.00442264	0.01764231	0.01057312
		7	4	7	1	2	8	5		1	3	2
0.05	0.95	22.6708	14.4029666	1.47571754	2.35171481	11.1525646	0.00045332	0.00139233	0	0.00502551	0.02106578	0.01428235
		5	7	6	8	7	3	8		6		2
0.1	0.9	29.2987	18.2334444	1.96109011	2.71629378	13.9704858	0.00054240	0.00173928	0	0.00578315	0.02530339	0.01890967
			4	5	4	6	4	2		9	6	5

Table A.13.1 Natural Gas-Diesel at 2000 K

Diesel	NO	O2	h for natural	h for diesel	h	h	Moles of O2	Moles of N2	Heat Release	Per unit of	Per Unit of
(kmol)			gas		nitrogen	oxygen			KJ	NO Formed	OH Formed
					gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.026550323	0.211278611	48644.11145	717902.5747	56130	59169	2.22222222	8.35555556	193175994.8	7275843540	11512626951
0.01	0.028347472	0.225645861	48644.11145	717902.5747	56130	59169	2.383055556	8.960288889	205956755.5	7265436303	11674022292
0.05	0.035536364	0.283119793	48644.11145	717902.5747	56130	59169	3.025833333	11.37713333	257035673.8	7233032350	12201574292
0.1	0.044522743	0.354969601	48644.11145	717902.5747	56130	59169	3.830555556	14.40288889	320983601.9	7209430085	12685396240

Table A.13.2 Natural Gas-Diesel at 2000K

T = 2500 K				Moles of Fuel per Mole of Product								
Diesel (kmol)	Natural Gas (kmol)	MW fuel	Air (kmol)	CO2	H2O	N2	Н	0	N	H2	ОН	СО
0	1	16.043	10.57777778	0.806455486	1.853602801	8.310897227	0.023409962	0.025964698	2.94311E- 06	0.073150391	0.123083418	0.193544396
0.01	0.99	17.36857	11.34334444	0.886147877	1.920854354	8.870717977	0.024544257	0.027754489	3.13389E- 06	0.07551624	0.129545897	0.21185215
0.05	0.95	22.67085	14.40296667	1.205167555	2.190277496	11.11000028	0.029058551	0.03491104	3.89698E- 06	0.085121788	0.155142614	0.284832321
0.1	0.9	29.2987	18.23344444	1.604276659	2.526967145	13.90910747	0.034664781	0.043853164	4.8508E- 06	0.097316926	0.18676702	0.375723497

Table A.14.1 Natural Gas-Diesel at 2500 K

Diesel	NO	O2	h for natural	h for diesel	h	h	Moles of O2	Moles of N2	Heat Release	Per unit of	Per Unit of
(kmol)			gas		nitrogen	oxygen			KJ	NO Formed	OH Formed
					gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.089313123	0.273012348	96962.12404	1112667.175	74305	78346	2.22222222	8.35555556	241550507.2	2704535448	1962494311
0.01	0.095583546	0.29295925	96962.12404	1112667.175	74305	78346	2.383055556	8.960288889	257531459.8	2694307460	1987955360
0.05	0.120661178	0.372753234	96962.12404	1112667.175	74305	78346	3.025833333	11.37713333	321400103.1	2663657934	2071642954
0.1	0.152004059	0.472510521	96962.12404	1112667.175	74305	78346	3.830555556	14.40288889	401360032.6	2640456017	2148987721

Table A.14.2 Natural Gas-Diesel at 2500 K

T = 3000 K				Moles of Fuel per Mole of Product								
Diesel (kmol)	Natural Gas (kmol)	MW fuel	Air (kmol)	CO2	Н2О	N2	Н	О	N	Н2	ОН	СО
0	1	16.043	10.57777778	0.359540532	1.303145373	8.240626685	0.318289208	0.262520644	0.000141918	0.321911623	0.432031956	0.640459468
0.01	0.99	17.36857	11.34334444	0.395853172	1.348224514	8.795474355	0.333345614	0.280698101	0.000151233	0.331631728	0.459182754	0.702146895
0.05	0.95	22.67085	14.40296667	0.541598474	1.528538576	11.01483922	0.393190808	0.353427742	0.000188651	0.371185665	0.542361042	0.948401526
0.1	0.9	29.2987	18.23344444	0.724459046	1.754011375	13.78901805	0.467416789	0.444367847	0.000235575	0.421550143	0.651459613	1.255540855

A.15.1 Natural Gas-Diesel at 3000 K

Diesel	NO	O2	h for	h for diesel	h	h	Moles of O2	Moles of N2	Heat Release	Per unit of	Per Unit of
(kmol)			natural gas		nitrogen	oxygen			KJ	NO Formed	OH Formed
			_		gas	gas				(KJ/kmol)	(kJ/kmol)
0	0.229715311	0.428962795	148214.797	1652274.501	92730	98036	2.22222222	8.35555556	289931183.2	1262132604	671087356.3
0.01	0.245924917	0.460623085	148214.797	1652274.501	92730	98036	2.383055556	8.960288889	309113980.4	1256944533	673182904.7
0.05	0.31080073	0.587470217	148214.797	1652274.501	92730	98036	3.025833333	11.37713333	385778959	1241242126	711295482.4
0.1	0.391948881	0.746320824	148214.797	1652274.501	92730	98036	3.830555556	14.40288889	481759154.5	1229137720	739507323.2

A.15.2 Natural Gas-Diesel at 3000 K