



Prospects of a Sootless Diesel Engine through use of Alcohol Fuels

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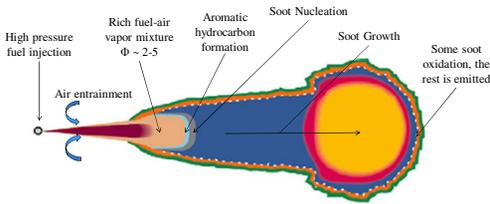
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Motivation and Background

Emission of soot, or solid-phase carbonaceous particulate matter, is of concern for two main reasons: public health due to its possible carcinogenic properties, and its impact on global warming. This work aims to investigate the prospect of eliminating engine-out soot emissions from direct injection Diesel engines.

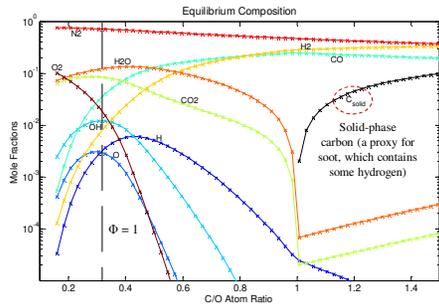
Soot emission is prevalent in Diesel engines in part because of locally high equivalence ratios (i.e. lack of oxygen) within the injected fuel jet. This leads some of the fuel down a chemical pathway where the cracked fuel species (small hydrocarbons like ethylene, C_2H_4 , and acetylene, C_2H_2) cannot oxidize. Instead they form aromatic rings, beginning with benzene ($A1-C_6H_6$), and once the rings are large enough are capable of "sticking" together and thus nucleating a solid phase.



A model of a quasi steady-state fuel jet from John Dec of Sandia National Laboratory. Using laser sheet imaging, he postulated that aromatic hydrocarbons form and then condense into soot just downstream of a premixed fuel-air vapor region.

Chemical kinetic limitations is the primary reason why soot formation occurs and the fuel does not fully oxidize. The progress towards equilibrium is halted due to the population growth of aromatic species and their subsequent dimerization.

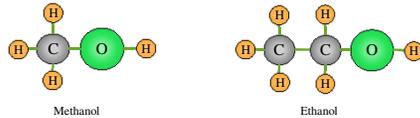
If equilibrium were reached, then unless the region is very oxygen insufficient, the products will be composed of mostly carbon monoxide (CO) and hydrogen gas (H_2). These species can then oxidize in the outer diffusion flame surrounding the jet, producing sensible energy for work extraction and forming low chemical energy combustion products of water (H_2O) and carbon dioxide (CO_2), and not soot.



Thermodynamic equilibrium products of a pre-mixed n-heptane (Diesel fuel surrogate) and air mixture, with initial temperature $T_i = 1000$ K. Equilibrium is constrained to constant enthalpy and pressure, approximating the environment of a mixed fuel-air parcel within the jet.

It is a goal of this research to understand how to reach equilibrium within the jet without becoming kinetically limited and forming soot.

Use of Alcohols



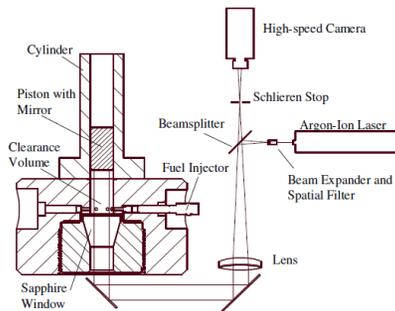
Alcohols, specifically methanol and ethanol, provide a good starting point for this research for a few reasons:

- Unlike Diesel fuel (which is a blend of many different hydrocarbons) they have well known compositions (i.e. atomic ratios).
- Research has been conducted on their autoignition characteristics, and chemical mechanisms exist that aim to predict their combustion behavior.
- They are oxygenated species, which helps to reduce the burden of air entrainment on decreasing the equivalence ratio locally within the fuel-air vapor region.
- They are miscible with water. This provides a simple means for bringing additional oxygen atoms into the mixture without relying on air entrainment.
- Production of ethanol as a bio-fuel is already taking place and is expected to grow in the near future. This is especially true if cellulose methods of production become more viable.

Experimental Apparatus

Chemical kinetics have a non-linear dependence on temperature. In order to avoid kinetic limitations (e.g. long lifetimes of large aromatic species), it is necessary to create high enthalpy air into which fuel may be injected, mixed, and combusted. An extreme compression, free-piston device is used to create such an environment within the lab.

Optical access is achieved through the use of a sapphire window at the bottom of the combustion chamber. By beaming an argon-ion laser through the combustion chamber and off of a mirror placed on the piston face, Schlieren imaging allows the observation of the fluid mechanics of rapid air compression, fuel injection, air entrainment and plume dilatation due to combustion.



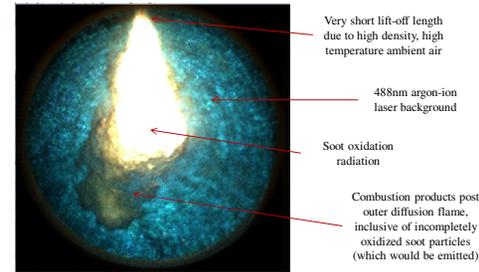
A high pressure air reservoir (not shown above) is used to drive the free-piston down the cylinder, achieving geometric compression ratios up to 100:1. This is a single-shot device, and does not have conventional intake or exhaust valves. Image courtesy of Matt Svreck.

Image Results

The Phantom high-speed camera is capable of taking color images every 28 μs (~36,000 frames per second) with a maximum exposure time of 26 μs . This allows for very sensitive detection.

The spatial observation of soot oxidation is easy due to its luminosity in the visible wavelengths (i.e. yellow emission).

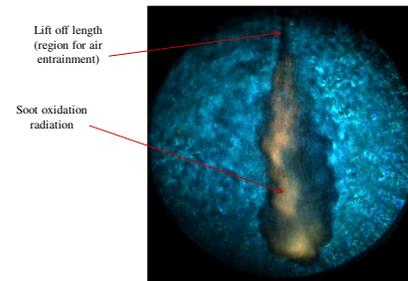
Reference Diesel #2 Fuel Injection



The above image was taken at the peak combustion chamber temperature and pressure, referred to as Top Dead Center (TDC), with a compression ratio of ~ 58:1. This corresponds to an ambient air environment of 255 bar and 1295 K. The injection of fuel began 1.5 ms prior to the image, and the exposure time was 3 μs .

Methanol Injection

Experimentation with methanol injections have produced a very interesting result: within the fuel jet, methanol does in fact form soot particles!



The above image was taken at TDC for a compression ratio of ~ 46:1. This corresponds to ambient air conditions of 185 bar and 1195 K. The injection of fuel began ~ 1 ms prior. The exposure time of the image is 26 μs , a factor of 9 times longer than the exposure time shown for the reference Diesel fuel above.

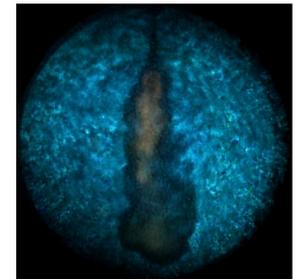
This result is rather unexpected. The common understanding of methanol direct injection combustion is that engine-out emissions do not include soot particles. While this imaging study does not refute that, it does indicate that soot particles do form within the jet. The volume fraction of soot particles is likely so small that it is able to completely oxidize before being emitted from the cylinder. Further research on a single-cylinder reciprocating engine within our laboratory is currently underway to verify this postulate.

Working Towards Eliminating Soot Formation

Direct injection of methanol into high pressure and temperature environments has been shown to form soot. Thus, this is a good fuel for investigating with water mixtures, changing local atom ratios (namely oxygen content), and potentially controlling the chemical pathways that the combustion process follows.

Methanol-Water Mixture Injection

A mixture of 4:1 moles of methanol to water is prepared. This corresponds roughly to 10% of water by volume.



The above image was taken at TDC for a compression ratio of ~ 47:1. The injection of fuel began ~ 1 ms prior. The exposure time of the image is 26 μs . This is approximately the same time and environment as the neat methanol injection image shown to the left.

It is observed that less soot has formed since a smaller spatial extent of the plume is showing visible luminosity. There are two possible mechanisms:

- Thermal effects: the water's enthalpy of vaporization has reduced the temperature of the fuel-water-air mixture just downstream of the liquid region of the jet. This subsequently reduces the peak temperature of combustion, which may contribute to a reduction in soot particle formation.
- Chemical effects: the water could be dissociating, contributing oxidizing OH radicals and allowing the cracked fuel to go through oxidation rather than cyclization (i.e. forming aromatic ring soot precursors), thereby reducing the amount of soot formed.

It is the chemical effect that is desirable. In this case, the water participates as a moderator species allowing the fuel to reform primarily into CO and H_2 , combustion temperatures are kept high, and high work output from the engine is maintained.

Next Steps

Presently, a number of efforts are underway to continue our understanding of how an in-plume fuel reformation process can occur:

- Continuing with wet methanol mixtures, we aim to find under what conditions the water will dissociate enough to participate in the chemical reactions. This can be accomplished by using higher compression ratios, as well as pre-heating the uncompressed air and thus reaching much higher peak temperatures due to nearly isentropic compression.
- Numerically, we are using chemical kinetic mechanisms that include aromatic hydrocarbon species that help indicate soot forming tendencies.

Additionally, a separate single-cylinder reciprocating engine is being used to gather performance and emissions data for both methanol and ethanol direct injection. A smoke meter is used to measure cylinder-out soot quantity, as a function of operating conditions (equivalence ratio, injection pressure, etc.).

Special thanks to GCEP (Global Climate Energy Project) for funding this research, and to Scott Sutton and Ken Hencken for operational support, as well as BJ Johnson for support with the Proteus engine.