Title: Analysis of SI Engine Alternative Fuels for Mixture Formation Behavior Related to Particulate Matter Formation with a Representative Gasoline Surrogate: Application to 2-Methyl-3-Buten-2-ol (Methyl Butenol, MBO)

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Project Goals:

The goal of this project is to develop a screening process based on component properties to determine whether the performance of new potential biofuels, such as 2-methyl-3-buten-2-ol (methyl butenol, MBO), when blended with gasoline, meet or exceed the performance of biofuels already established in the market, such as ethanol and isobutanol (IBA). The screening process will include properties important to spark-ignition direct-injection (SIDI) engines related to mixture formation, combustion, and particulate matter (soot) emissions. To assess biofuels that are available in limited quantities the screening process must be done computationally to minimize time and resources. To computationally screen biofuels for properties when blended with a gasoline, a representative gasoline surrogate was developed to accurately model and estimate properties of gasoline-biofuel blends.

Abstract Text:

Ethanol and isobutanol (IBA) have seen significant study of their engine performance when blended with gasoline. Recently, the terpene compound 2-methyl-3-buten-2-ol (methyl butenol, MBO) was identified as a potential gasoline blending component that may have favorable properties. To assess this, we consider biofuels blended with a gasoline blendstock for oxygenated blending (BOB), a gasoline with lower octane number that is used specifically for blending with oxygenated biofuels. Early efforts focus on estimation of gasoline-biofuel blend properties determined that the computational gasoline surrogate composition had a significant impact on these estimates. To address this, a new surrogate formulation methodology was developed that targeted matching of the chemical composition of the gasoline as well as the distillation curve (volatility), research octane number (RON) and motored octane number (MON) (autoignition), and hydrogen-to-carbon ratio (H/C) (flame speed and adiabatic flame temperature). With the new methodology, the surrogate composition matches the reference gasoline with less than 1.5% error in n-alkanes, iso-alkanes, and aromatics mole fractions. The error for other quantities is also low with average root mean-squared error for the distillation curve of 3.1% and errors for RON, MON, and H/C all less than 1.5%. The new surrogate formulation method also allows for identification of additional surrogate compositions that may have similar overall error but match particular properties better that were not included directly in the optimization process.

The reminder of this work focuses on screening properties of MBO related to in-cylinder mixture preparation in spark-ignition direct-injection (SIDI) engines that may impact particulate matter (PM) formation. The proposed screening parameters include the equilibrium distillation curve (EDC) and standard enthalpy requirement (SER). These parameters were calculated for MBO-, IBA-, and ethanol-gasoline blends at fuel matched oxygen weight percentages of 4, 7.5, and 11%. The results of the distillation curve calculation show an increase in aromatic component concentration at the 90% distillation point for ethanol at all blend percentages. For MBO and IBA the mole fraction of oxygenate increases at the 90% distillation point with increasing oxygenate weight percent, whereas for ethanol it remains almost constant. A redefined SER calculation showed that the energy needed to vaporize the fuel increases significantly with oxygen weight percent for addition of IBA and ethanol, while it remains almost unchanged for MBO. Combined, the results help explain the increased PM emissions seen from SIDI engines operating on ethanol-gasoline blends under certain operating conditions. The results also indicate that MBO will likely not suffer from this issue and may reduce PM emissions in general.

References/Publications

1. Shen, A., Sakai, S. & Rothamer, D. "Parameters for screening SI engine alternative fuels for mixture formation behavior related to particulate matter formation: application to 2-methyl-3-buten-2-ol (methyl butenol, MBO)." in Spring Technical Meeting of the Central States Section of the Combustion Institute. (2020).
2. Shen, A. “Parameters for screening SI engine alternative fuels for mixture formation behavior related to particulate matter formation: Application to 2-methyl-3-buten-2-ol (methyl butenol, MBO).” ACS Fall 2020 Virtual Meeting & Expo, 17-20 Aug. 2020, online.

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