An Investigation into the Potential of Biomass Derived Fusel Alcohol Mixtures for Improved Engine Performance

University of Dayton

Lily Behnke

Advisor: Joshua Heyne, Ph.D.

Research Objective: To implement biomass derived renewable fusel alcohol blends as an alternative fuel source to improve upon traditional gasoline properties for increased engine performance

Motivation

- In 2017, greenhouse gas concentrations reached new heights with a globally averaged mole fraction of CO_2 at 405.5 parts per million (ppm) [1]
- This crisis is reflected in the affordable and clean energy and climate action goals for the UN's 2030 sustainability agenda[2]

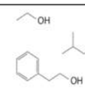
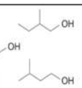
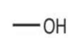
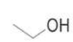
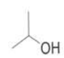
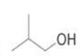
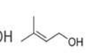
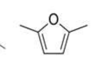
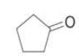
Background

- Co-cultures of engineered strains of E. coli and Corynebacterium were used for the systematic production of fusel alcohols from algae strains and distillers grains[3]
- The Merit Function, below, calculates a unitless comparison to represent the expected thermodynamic efficiency gain compared to the national average gasoline

$$Merit\ Score = \left(\frac{RONmix-91}{1.6}\right) - (K(OSmix)-8) + (0.085[ON]((\left(\frac{HoVmix}{AFRmix+1}\right) - ((415/(14.0+1)) + \left(\left(\frac{HoVmix}{AFRmix+1}\right) - \frac{\frac{415}{14.0[-]+1}}{15.2}\right) - H(PMImix - 1.6)[0.7 + 0.5(PMImix - 1.4)]$$

Methodology

- The Merit Function only takes into account efficiency properties, however other properties such as energy density and vapor pressure are still of importance to fuel refineries and consumers
- Fusel alcohol blends demonstrate beneficial efficiency properties as well as high energy density and low vapor pressure values as seen in columns 1 & 2 of the table below
- A computational matrix of potential blends of fusel alcohols was developed to evaluate the Merit Score and properties beyond the scope of the Merit Function

Strong Performance / Good Performance / Marginal Performance / Poor Performance	Algae Fusel Alcohol Blend	Distillers Grains Fusel Alcohol Blend	Methanol	Ethanol	Isopropanol	Isobutanol	Prenol	Diisobutylene	Furan Mixture	Cyclopentanone
Chemical Structure										
Blending RON	127	126	143	130	122	109	140	130	146	125
Octane Sensitivity	32	31	44	35	17	25	38	29	41	22
Heat of Vaporization [kJ/kg]	691	691	1173	919	744	508	508	318.2	355	504
Particulate Matter Index	1.8	2.0	0.05	0.06	0.08	0.17	0.17	0.57	0.57	0.74
Sooting index	32.7	32.7	6.6	10.3	19.2	26.2	26.2	68.5	NA	22
Merit Function Score at 20 vol%	4.7	4.2	11.9	9.1	2.7	4.2	6.6	4.5	8.8	3.4
Energy Density [MJ/kg]	35.2	35.2	20.1	26.8	30.7	33.1	34.4	44.3	34	32
Blending Vapor Pressure	Low	Low	High	High	High	Moderate	Low	Low	-	-
Water solubility [g/L]	237	215	1000	1000	1000	85	17	0.004	2.2	60.8
Stability Issues	Minimal	Minimal	Minimal	Minimal	Minimal	Minimal	Significant	Significant	Severe	Moderate
Infrastructure Compatability	Moderate	Moderate	Poor	Poor	Poor	Moderate	Moderate	Moderate	Moderate	Very Poor

The table above shows the properties of fusel alcohol blends compared to the biomass derived fuels with the highest Merit Scores as determined by the Co-Optima program and Sandia National Laboratories.

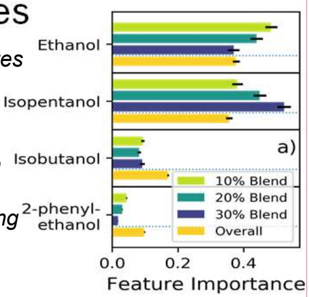
References

1. "Greenhouse gas concentrations in atmosphere reach another height", World Meteorological Organization, 2020.
2. "Sustainable Development Goals Knowledge Platform", United Nations, 2018
3. Katherine DeRose, Fang Liu, Ryan W. Davis, Blake A. Simmons, and Jason C. Quinn *Environmental Science & Technology* 2019 *53* (17).

Results

- Random Forest Regression Analysis was used to measure the relative feature importance of each fuel with respect to the Merit Score
- Ethanol's feature importance decreases with blending percentage while isopentanol's increases

Ethanol contributes less to efficiency gains at higher blending percentages with gasoline while linearly decreasing energy density



Conclusions

- Pure Ethanol is not necessarily the "best" solution at higher blending percentages, fusel alcohol blends increase energy density and decrease vapor pressure while maintaining a high Merit Score