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Leveraging the benefits of ethanol in advanced engine-fuel systems

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ABSTRACT

Ethanol is one of the most desirable fuels for spark-ignition engines. It offers high-octane quality and a latent heat of vaporization that is four times greater than gasoline on a stoichiometric basis. Anhydrous ethanol can also readily be blended into oil-based fuels, thereby enabling improved engine efficiency and reduced greenhouse gas (GHG) emissions. However, the use of ethanol is currently constrained by low yield production processes and a reliance on considerable amounts of arable land to cultivate the most widely utilized feedstocks. These challenges could be addressed if ethanol was instead derived synthetically from petroleum-based feedstocks. This paper presents a comparative well-to-wheel assessment for three different engine-fuel systems that leverage the benefits of ethanol which has been derived synthetically and from the fermentation of biomass. In the baseline case, anhydrous ethanol (99.5% by volume) derived from corn is used to produce a high-octane E30 gasoline (RON 101). The alternative case considers synthetic hydrous ethanol (~90% by volume) which is derived from direct hydration of ethene in a crude oil refinery. Hydrous ethanol is immiscible in gasoline, and is therefore utilized as a high-octane fuel for the Octane-on-Demand concept. The same engine-fuel system operated on anhydrous bioethanol is also considered for comparative purposes. Single cylinder engine tests are first used to characterize the specific fuel consumption and CO_2 emissions for the different engine-fuel systems. This data is then used to construct fuel consumption maps to simulate the drive cycle fuel economy of a light-duty vehicle. Finally, the well-to-wheel GHG emissions are computed, with consequent uncertainties assessed using Monte Carlo analysis. The results demonstrate that the well-to-wheel GHG emissions for the three different engine-fuel systems are generally comparable. This is despite the Octane-on-Demand cases offering improved drive cycle fuel economy with respect to the E30 gasoline. These outcomes are shown to be largely insensitive to uncertainties in the upstream fuel production GHG emissions. Overall, this suggests that the use of synthetic ethanol in advanced engine-fuel systems could supplement bioethanol derived from first and second generation feedstocks in the future transport energy mix.

1. Introduction

Ethanol has become an important blend component in the oil refining industry, with an estimated 13.7 billion gallons blended into gasoline in the United States in 2015 [1]. Ethanol has a high-octane number (RON ~109) and a latent heat of vaporization (HoV) that is four times greater than gasoline on a stoichiometric basis [2,3]. These characteristics enhance the anti-knock quality of oil-based fuels [4–7], thereby enabling improved engine efficiency and reduced greenhouse gas (GHG) emissions [8–12].

The majority of global ethanol production (~93%) currently involves the fermentation of biomass [13]. The remaining ethanol is synthetically produced from petroleum-based feedstocks, with the most widely utilized process involving direct hydration of ethene [14–16]. This process takes place at around 500 K and 7 MPa in the presence of an acidic catalyst (Reaction (1)). Each pass of the reactor converts around 5% of the ethene to ethanol. The unreacted ethene is then separated and recycled back into the reactor. The final product is chemically identical to bioethanol, and can only be distinguished by radiocarbon dating [17].

$$CH_2 = CH_2 + H_2O \rightarrow CH_3CH_2OH \quad (1)$$

Producing ethanol synthetically may offer several advantages over the fermentation of biomass. Firstly, synthetic ethanol can be produced alongside conventional transport fuels in a crude oil refinery. The production process is also continuous, high yield (~95%) and high purity [18,19]. By contrast, bioethanol generally involves low yield (~12–20%) batch processes and requires additional steps to remove impurities [20]. Considerable amounts of arable land are also required to cultivate the most widely utilized feedstocks, which is often obtained

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Nomenclature

aTDC	after top dead center
BMEP	brake mean effective pressure
BOB	blendstock for oxygenated blending
BSFC	brake specific fuel consumption
CA50	crank angle at which 50% of the fuel mass has been burned
CO_2	carbon dioxide
CO_2-e	CO_2-equivalent emissions
CH_4	methane
DEF	diesel exhaust fluid
DI	direct injection
E22	fuel composed of up to 22% ethanol by volume
E30	fuel composed of up to 30% ethanol by volume
E85	fuel composed of up to 83% ethanol by volume
EGR	exhaust gas recirculation
EtOH	ethanol
FFV	flex-fuel vehicle
g CO_2/km	grams of carbon dioxide per kilometer
g/kW h	grams of fuel consumed per kilowatt hour
GHG	greenhouse gas
GREET	greenhouse gases, regulated emissions, and energy use in transportation model
H-EtOH	hydrous ethanol
H/C	hydrogen-to-carbon ratio
HoV	heat of vaporization
IMEP	indicated mean effective pressure
kW	kilowatts
L/100 km	liters of fuel consumed per 100 km
LCFS	Low Carbon Fuels Standard (California)
LHV	lower heating value
LUC	land use change
MBT	minimum spark advance for best torque
Min. FC	minimum combined fuel consumption
MON	Motor octane number
NO	nitric oxide
N_2O	nitrous oxide
Nm	Newton meters
NMEP	net mean effective pressure
NO_x	nitrogen oxides
$NSCO_2$	net specific carbon dioxide emissions
NSFC	net specific fuel consumption
OoD	Octane-on-Demand
P10	tenth percentile
P50	fiftieth percentile (median value)
P90	ninetieth percentile
PDF	probability distribution function
PE	peak efficiency
PFI	port-fuel injection
PM	particulate matter
RFS2	Renewable Fuel Standard 2
RON	Research octane number
rpm	revolutions per minute
SG	specific gravity
TTW	tank-to-wheel
US06	Supplemental Federal Test Procedure
% v/v	volume fraction
% w/w	weight fraction
WLTP	Worldwide harmonized Light vehicles Test Procedure
WTT	well-to-tank
WTW	well-to-wheel
λ	relative air-fuel ratio

through deforestation [21,22]. More recently, concerns have also been raised in relation to declining soil fertility, excessive water consumption, and the increased use of fertilizers and harmful pesticides (eutrophication) [23–33].

These factors have contributed towards renewed interest in synthetic ethanol. Countries such as Brazil, the second largest global producer of bioethanol, regularly import synthetic ethanol when their domestic sugarcane harvests decline due to changes in weather conditions and cropping patterns [34,35]. Similarly, the largest source of imported ethanol for the United States until the mid 2000s was Saudi Arabia Basic Industries Corporation (SABIC), which produced the ethanol from surplus ethene in petrochemical facilities [36]. China has also recently expanded its synthetic ethanol production to around 8% of total capacity, but has instead favored acetic acid hydrogenation technologies due to the country's vast coal resources [37]. China's synthetic ethanol production capacity is expected to grow to 1104 million liters by the end of 2017; an annualized increase of 30% [38].

Irrespective of whether ethanol is produced synthetically or from the fermentation of biomass, the resulting mixture contains excess water [39]. The ethanol is extracted from this mixture using distillation, which yields a hydrous ethanol mixture composed of up to 95.6% ethanol by weight (~93% by volume). This azeotrope can be used as a fuel in flex-fuel vehicles (FFV), but is immiscible in gasoline due to the high water content [40–43]. The mixture must therefore be dehydrated so that it contains a maximum of 1% water by volume to be suitable for gasoline blending [44]. This involves costly and energy intensive processes such as molecular sieve adsorption [45,46]. As a result, the use of hydrous ethanol with even 5% water by volume could provide considerable cost and energy savings [47–49].

The combustion of hydrous ethanol has been studied in a wide range of engine applications. Aside from the common concerns related to miscibility, most studies have reported that hydrous ethanol is generally beneficial for both engine efficiency and nitrogen oxide (NO_x) emissions [50–54]. Hydrous ethanol can also reduce particulate matter (PM) and nitric oxide (NO) emissions in compression ignition engines [55,56]. Other benefits of hydrous ethanol may include reduced vehicle operating costs for consumers. For example, Lanzanova et al. [57] estimated that lean engine operation with 10% water in ethanol (by volume) provided cost reductions of up to 31% with respect to anhydrous ethanol under stoichiometric engine operating conditions. The retail price of hydrous ethanol in places such as Brazil is typically 70% of gasoline [58].

However, these benefits are offset by an increase in the specific fuel consumption due to the lower energy density of hydrous ethanol mixtures (Fig. 1). This is particularly problematic for mixtures with significant water content [59–62], and suggests that the net environmental impact of hydrous ethanol could actually be similar to conventional

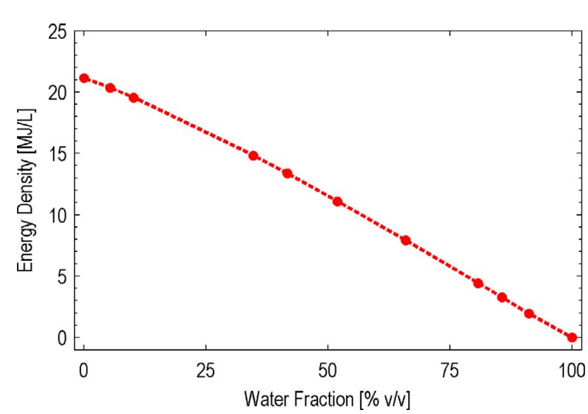

Fig. 1. Energy density of binary ethanol-water mixtures.