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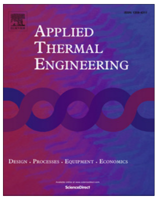

Research Paper

Modelling of evaporative losses in n-alcohol/diesel fuel blends

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HIGHLIGHTS

- Modelled evaporative losses from blends agreed with experimental results.
- Diffusion and activity coefficients were proved to have significant effect.
- Evaporation rate was proportional to the decrease in the alcohol carbon number.
- Paradoxically, evaporative losses are faster in blends with lower alcohol content.

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ABSTRACT

Alcohol/diesel fuel blends allow reducing the formation of soot in diesel engines. However, its use in a large scale framework still faces the challenge of high evaporative losses under storage conditions which is hindered by the high volatility of the alcohols. Since the design of the most adequate fuelling system for each blend requires detailed knowledge about the evaporation losses from the liquid phase, in this work a method for calculating the evaporation of pure n-alcohols (from C1 to C5 carbon atoms) and blends of these alcohols with ultra-low sulphur diesel (ULSD) was proposed. Alcohols vapour pressure was determined with the Antoine equation, while the diffusion coefficient of alcohols in air was calculated as a function of carbon number and temperature. The coefficients of activity were obtained by the combination of continuous thermodynamic (gamma distribution function) and a modified UNIFAC-Dortmund-Continuous method. The evaporation losses model is based on Fick's law and exhibited good agreement with experimental data for all alcohols and blends at 20% content of all alcohols and at 20–60% contents of n-butanol with diesel fuel. The evaporation was found to decrease approximately with an inversely proportional rate with respect to the increase in the carbon chain length of the alcohol. The paradox of faster evaporative losses from blends with lower alcohol content is explained.

1. Introduction

Blending diesel fuels with bioalcohols is one of the most efficient means to introduce a renewable fraction in the fuel, to improve its sustainability, and to provide some oxygen content, this being essential to reduce soot engine emissions. Additionally, compared with biodiesel/diesel blends, alcohol/diesel (or even alcohol/biodiesel/diesel blends) can provide similar renewable fraction, similar oxygen content and superior soot-reduction potential with much lower cost and energy consumption. The hydroxyl group of the alcohol molecules contributes to reduce soot formation, and consequently particulate emissions, even more than other functional groups with the same oxygen content [1–3], especially at high engine loads [4,5]. However, different challenges will have to be faced for the future extension of the use of these alcohols as diesel fuel components to a large scale.

First, the energy and environmental life-cycle assessments of the bioalcohols must be advantageous with respect to other biofuels. The recent commitments to further reduce greenhouse emissions from transportation sources make this a crucial factor. Ethanol has proved to have a significant potential for reducing life-cycle greenhouse gas emissions, as acknowledged by the European directive 28/2009/CE [6], where the typical greenhouse savings range from 21% (in the case of using wheat as feedstock) to 75% (in case of sugar cane ethanol) or even to 87% (in case of wheat straw). Methanol is also gaining interest as a renewable fuel, since its production derived from gasification of waste biomass followed by catalytic synthesis at high pressure provides both high yield (45–55% in weight) and energy efficiency (70–75%) [7]. Biomass

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Nomenclature

A	area of the cylindrical vessel
A, B and C	coefficients of the Antoine equation
D	diffusion coefficient
d	diameter of the cylindrical vessel
f	fugacity
H_r	mean relative humidity
L	free height of the vessel with respect to the liquid interphase
$\dot{m}$	mass flux
m''	mass flux per area
n	number of carbon atoms
p	pressure
R	gas constant
T	temperature
t	time
V	volume
v	mole volume
W	molecular weight
w	mass fraction
x	mole fraction
z	volume fraction, compressibility factor, height
ϕ	coefficient of fugacity
γ	activity coefficient
ρ	density

Subscripts

A	alcohol
Air	air
b	boiling
c	critical
D	diesel fuel
i	instant
L	free height of the vessel
0	interphase ($z = 0$)
v	vapour

Superscripts

l	liquid
v	vapour

sources are even preferable for biomethanol production than for bioethanol because the last is a high-cost and low-yield product [8,9]. Butanol has also proved to have an interesting potential for saving life-cycle greenhouse emissions when it is produced from acetobutylicum fermentation, as far as the bio-acetone obtained as co-product is valued as such [10]. Other higher alcohols could also become a sustainable alternative as far as they can be produced in biorefineries together with a wide range of commodities.

Second, the fuel storage and handling difficulties derived from the high volatility of alcohols must be addressed. Previous experiences with ethanol–diesel blends have proved that different technical modifications in the fuelling system are necessary, such as the installation of seals for fuel tanks, security valves on both vehicle fuel tanks and fuel station tanks, and special systems for recovering of fuel vapours on vehicles and fuel stations and to avoid vapour locks. These restrictions constitute a barrier for the massive use of these blends in private vehicles, and have limited their practical use to captive fleets, such as those of urban buses or public construction and civil machinery.

Third, some key properties of the alcohol blends affecting the injection system may limit their use beyond certain limits. A previous work was published studying blending stability, lubricity, viscosity and cold filter plugging point as the key properties of alcohol–diesel blends [11].

Finally, among the properties affecting the combustion process, cetane number is certainly the most limiting one. Although diesel engines need to be fuelled with high cetane number-fuels (above 51 as stated by norm EN 590) to facilitate autoignition and provide short ignition delay, alcohols exhibit low cetane numbers [12,13]. For this reason, the direct use of alcohols as fuels for unmodified diesel engines is not recommended, unless they are blended with diesel fuel. However, long-chain alcohols have higher cetane number than short-chain alcohols [14,15], this enhancing their interest for being used in diesel engines.

The work presented here is related to the second challenge mentioned. The design of the most adequate fuelling system for each blend requires detailed knowledge about the evaporation losses from the liquid phase. This work proposes a model to predict evaporation losses from alcohols (from methanol to n-pentanol) blended with a diesel fuel under stagnant air conditions, and describes the guidelines to be followed for modelling evaporative losses from other base fuels and under more realistic evaporation conditions.

Although some literature has reported modelling studies on vapour pressure and evaporation losses in alcohol–gasoline blends [16] or in biodiesel–diesel blends [17], very few have been found addressing this issue in alcohol–diesel blends, and in any case, these studies have been applied to droplet evaporation in ethanol–diesel blends from combusting [18] or non-combusting [19] liquid sprays, rather than to evaporation losses from fuel storage systems.

2. Tested fuels, blends and experimental conditions

2.1. Pure fuels

The main measured specifications of pure alcohols and ULSD are shown in Table 1. The diesel reference fuel was supplied by the Colombian petroleum company (Ecopetrol). The alcohols used in this work were methanol (Honeywell, 99.9% purity), ethanol (Panreac, 99.5% purity), n-propanol (Merck, 99.5% purity), n-butanol (Panreac, 99.5% purity), and n-pentanol (Panreac, 98% purity).

2.2. Blends

Blends of 20% by volume of the five n-alcohols in ULSD fuel were selected to experimentally validate the evaporation model. Additionally, blends of n-butanol with 30%, 40%, 50% and 60% content in diesel fuel were also selected to study the effect of the alcohol content in the evaporation losses. The volume, mass and mole fractions of each alcohol (identified with subscript A) in each of the tested blends are shown in Table 2.

The 20% blends were selected because this concentration is high enough to modify the blend properties with respect to those of pure diesel fuel, and additionally, because they might be eventually of interest to be implemented in the market. For the study about the effect of the alcohol content, n-butanol was chosen because it presents good miscibility with diesel fuel at all