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Abstract - Introducing water with fuel in diesel engines has been proved to be powerful and economical method for reducing combustion pollutant emissions from the engine. Most studies available in literature discuss the effect of adding water to the fuel in the range 5 to 10% water. In this paper, results of modeling study are presented where the effect of relatively high water content in fuel has been investigated. The fuel used was a surrogate mixture composed of 70% n-Heptane and 30% Toluene with two water contents of 25% and 35% by volume. The modeling study was performed using the commercially available software CHEMKIN at diesel engine-relevant conditions. The results show that water, even at high percentages, still has the tendency to reduce pollutant emissions as its concentration increases. Also, fuel consumption was found to decrease by increasing water content. However, the tradeoff with CO and Unburned Hydrocarbons UHC emissions was maintained.

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THE EFFECT OF HIGH WATER CONTENT OF FUEL ON DIESEL ENGINE EMISSION

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The Effect of High Water Content of Fuel on Diesel Engine Emission

Abdulaziz H. El-Sinawi [α], Kifah Takrouri [σ], Omar Osta [ρ] & No'man Haimour [Ѡ]

Abstract - Introducing water with fuel in diesel engines has been proved to be powerful and economical method for reducing combustion pollutant emissions from the engine. Most studies available in literature discuss the effect of adding water to the fuel in the range 5 to 10% water. In this paper, results of modeling study are presented where the effect of relatively high water content in fuel has been investigated. The fuel used was a surrogate mixture composed of 70% n-Heptane and 30% Toluene with two water contents of 25% and 35% by volume. The modeling study was performed using the commercially available software CHEMKIN at diesel engine-relevant conditions. The results show that water, even at high percentages, still has the tendency to reduce pollutant emissions as its concentration increases. Also, fuel consumption was found to decrease by increasing water content. However, the tradeoff with CO and Unburned Hydrocarbons UHC emissions was maintained.

Keywords : water-in-fuel emulsion, pollutants reduction, diesel, surrogate fuel, combustion.

I. Introduction

The exhausted gaseous phase from diesel engines is usually composed of hundreds of chemical compounds and pollutants. High engine temperatures are usually involved in the exothermic reactions of fuel with air. With the existence of nitrogen and oxygen from air or fuel, nitrogen oxides NO_x and carbon oxides CO_x are among the major pollutants emitted by the combustion process. To a lesser extent, Unburned Hydrocarbons UHC and Volatile Organic Compounds VOC can also be emitted as well as many trace amounts of hazardous air pollutants. Due to the impact of these emissions on the environment, many countries are gradually strengthening the regulations related to these emissions. As a result, diesel engine designers are challenged with two often conflicting goals: reducing the engine emissions and at the same time improving its efficiency.

Recently, intensive research has been done worldwide on developing methodologies that reduce the diesel engine pollutant emissions. Many of these methodologies are focused on improvements in engine design. However, such improvements are usually costly and difficult to apply.

One method for pollutants reduction is to decrease the engine high temperature by bringing water into the combustion chamber. Water can be injected to the engine inlet manifold, directly injected to the combustion zone or can be injected in the form of water-in-diesel emulsion. Among these technologies, the use of water-in-diesel emulsions was reported to be the most efficient to reduce pollutant emissions as, in addition to other effects, water is injected directly into the combustion zone causing a larger decrease of the combustion temperature [1, 2]. Water-in-diesel emulsions can also be applied with virtually no additional costs.

The main reason for the reduction in pollutants emission in the use of water-in-diesel emulsion is the reduction in the combustion temperature. The reduction in the temperature itself is due to (1) vaporization of liquid water which decreases the internal energy and (2) increasing heat capacity due to having higher trapped mass of vapor. Moreover, water provides its improvements physically by enhancing mixing within the engine and chemically by reacting with the combustion gases. Also, water, which has a much lower boiling point than that of the surrounding diesel in the emulsion, suddenly and dramatically expands upon vaporization. This expansion increases turbulence and enhances the mixing between oxygen and fuel. This process is usually referred to as the micro-explosion process. Several researches reported that the emulsion combustion reactions are not simply kinetically controlled, but the turbulence inside the combustor has a considerable effect.

The water-in-diesel emulsions emit reduced amounts of particulate matters and soot. These emulsions also show better burning efficiency and therefore reduce fuel consumption without engine modifications. However, one limitation is the potential increase in CO and UHC production.

In practice, extensive research has been done on the use of water-in-fuel emulsions. Some water-in-fuel emulsions, such as the Aquazole formulation developed by TOTAL, are already in use today on a large number of vehicles in France and other countries in Europe. It has been claimed that this formulation brings about a reduction of up to 30% in NO_x and of up to 80% in soot [3]. Water-in-fuel emulsions have also been used on autobuses in some areas of China.

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In literature, high water content in diesel emulsions (more than 10%) was rarely discussed and needs to be thoroughly investigated [4, 5].

This study provides modeling analysis of emissions reduction obtained by using water-in-fuel emulsions with water ratios of 25% and 35% in volume. Surrogate fuel was used in this study as detailed kinetic and thermodynamic data can be available for selected surrogate fuels but not available for conventional diesel. Conventional diesel fuels are blends of several hundreds of individual components [6]. Surrogate fuels can be reasonably considered as simpler representatives of the chemically complex conventional diesel fuel in terms of performance and emissions behavior [6]. As one-component surrogate fuel may not accurately reflect the behavior of real diesel, surrogate fuels of more than one component are usually employed. However, a surrogate fuel should be prepared with the smallest possible number of components that provide the desired representation of the conventional diesel. Surrogate fuel composed of 70% n-Heptane and 30% Toluene was used in this study.

In most of the studies conducted with regard to water-in-fuel emulsions only NO_x and particulate matter were the emissions of concern [7]. Some recent studies investigated the CO and UHC emissions. In this study, emissions of CO, UHC, VOC and other compounds like propargyl, benzene and others were looked at as well as emissions of n-Heptane; one component of the surrogate fuel used.

II. Literature Review

This literature review is focused on the combustion studies where relatively high water content in fuel (20% and above) was used. There are inconsistent results reported in different studies where high water contents were used which reveal the need for further research on combustion of such emulsions. Lif et al. [3] reported that the typical water content of a diesel emulsion is between 10 and 20%. However, Nazha et al. increased the amount of water up to 50% and reported a 60% reduction in NO_x but noticed a slight increase in smoke emissions [9].

Park et al. [8] used water up to 40% in combustion tests and the general picture of pollutants reduction was maintained. However, small effects on CO and UHC emissions were reported. In another study [3], the NO_x and soot levels were significantly reduced for water contents between 15–45% but the CO and UHC emissions increased. Canfield [10] reported a significant pollutant emissions reduction with up to 45% water, by volume, in diesel. He reported that of six technologies evaluated for pollutants reduction, the water-in-diesel emulsion promises the easiest solution.

Matheaus et al. [6] used diesel having 20% water by mass in an experimental study to investigate the effect of water on the engine emissions and fuel consumption rate. He reported a 19% reduction in NO_x and 16% reduction in particulate matter. However, there was 42% increase in CO and 28% increase in UHC.

III. Modeling, Results and Discussion

In this study, the commercially available code CHEMKIN was used to investigate the combustion of the selected surrogate fuel (70% n-Heptane and 30% Toluene) with water content of 25 and 35% by volume. CHEMKIN contains an extensive database of temperature dependent properties and a built-in chemical reaction kinetics solver which is appropriate for detailed combustion calculations. CHEMKIN computation is performed using 393 species and 1,925 reactions. The Partially Stirred Reactor PaSR modeling approach was used in this analysis. PaSR can assess the extent of interactions between turbulence and chemical kinetics and therefore can provide information on how turbulence intensity inside a combustor will affect combustion [11].

The initial temperature and pressure for the computations are 900 K and 39 bar; respectively, with air as the oxidizer. The temperature and pressure values agree with the actual parameters of a real engine [6]. The fuel/air equivalence ratio was 0.8.

Fig. 1 shows typical profiles of some major exhaust emissions resulting upon combustion of the surrogate fuel with 25% water. Fig. 2 shows the emissions plotted against water mole fraction. Most of the data of this paper are plotted against water mole fraction in the exhaust gaseous phase being a better representing parameter.

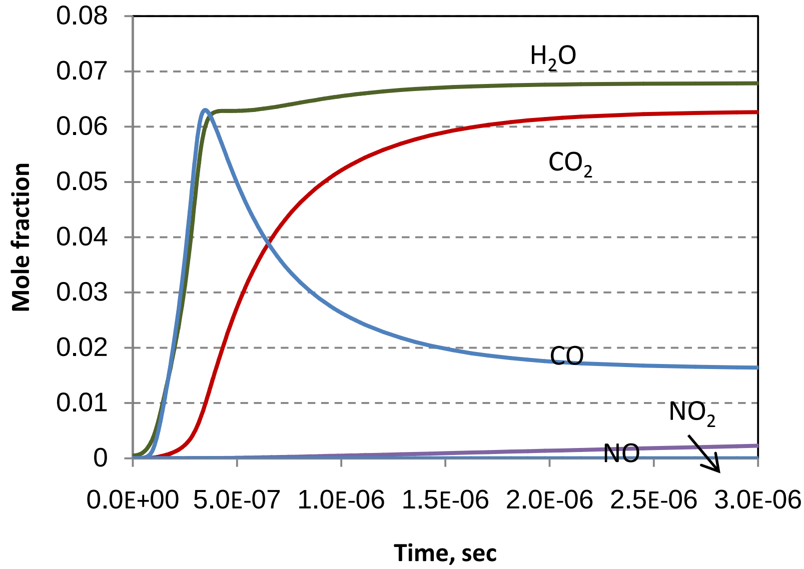

Fig. 1 : Typical NO_x, CO_x and water mole fraction profiles for 25% water content in emulsion of 70% n-Heptane and 30% Toluene.

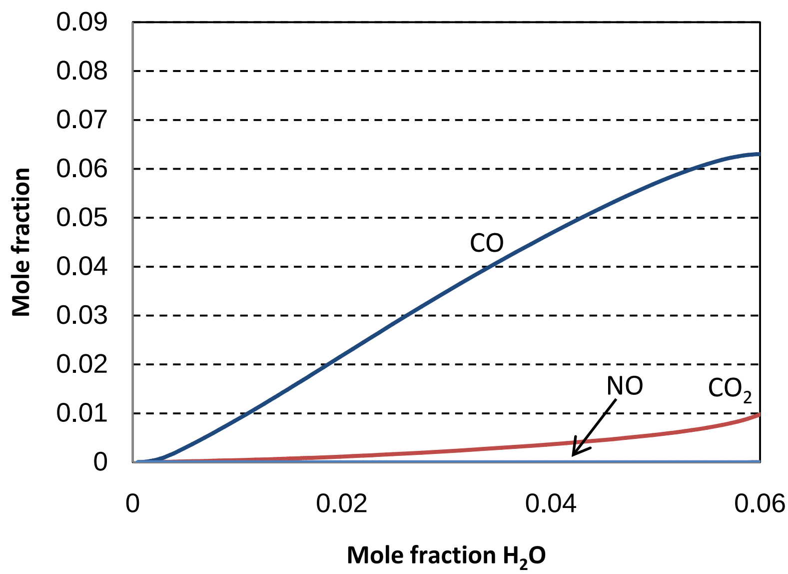

Fig. 2 : Typical plots of CO_x and NO mole fractions for 25% water content in emulsion of 70% n-Heptane and 30% Toluene.

Fig. 3 shows the calculated combustion temperature for the two water contents. As shown in the figure, the peak temperature decreases with increasing water content.

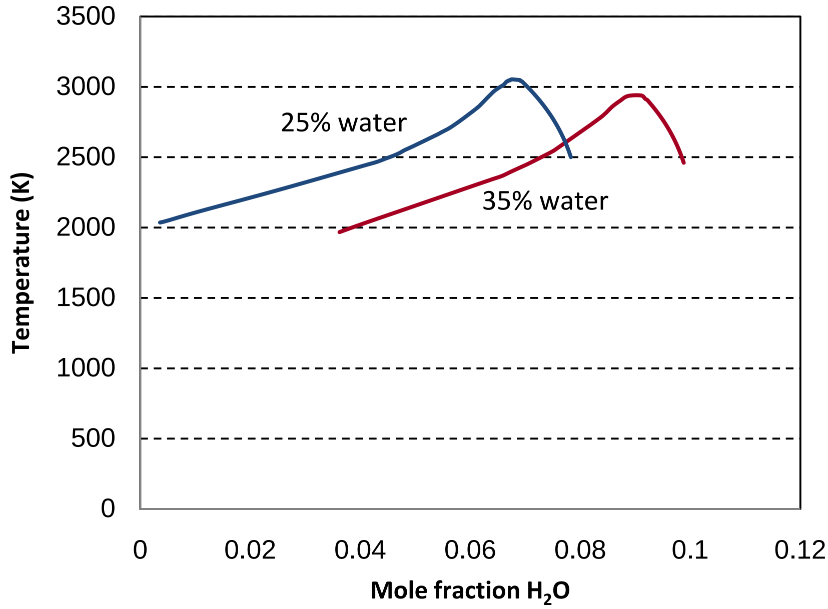

Fig. 3 : Calculated temperatures for 25% and 35% water in a surrogate fuel of 70% n-Heptane and 30% Toluene.

Fig. 4 shows the water mole fraction profile for the two emulsions. As expected, the water concentration in the exhaust gas is higher for the emulsion with higher water content.

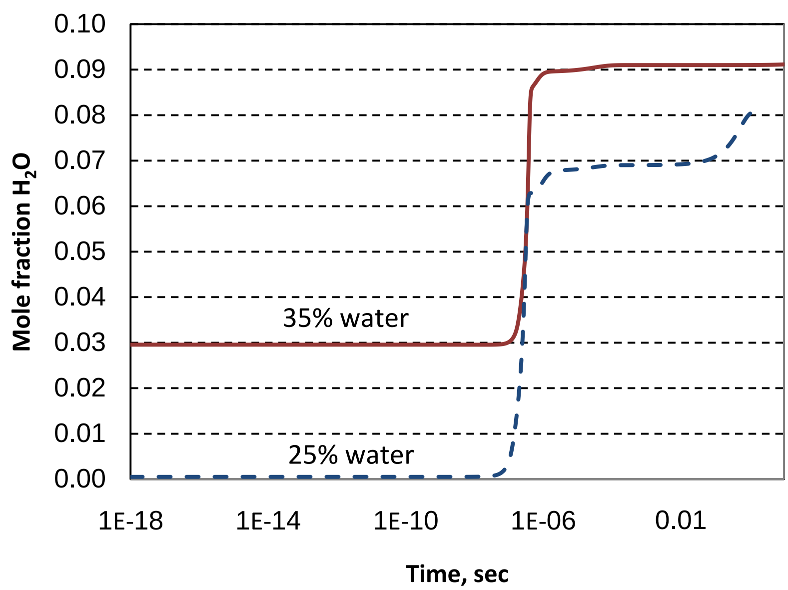

Fig. 4 : Water mole fraction profile for emulsions with water contents of 25% and 35% in a surrogate fuel of 70% n-Heptane and 30% Toluene.

Fig. 5 shows the mole fraction of n-Heptane for the two emulsions. The emulsion with the higher water content results in a higher n-Heptane concentration which is consistent with findings of other studies that increasing the water content may decrease the fuel consumption [3, 10, 12].

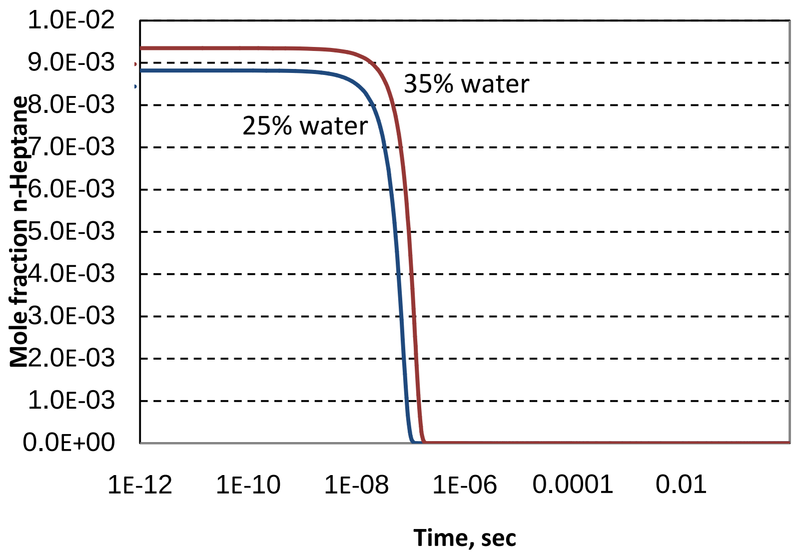

Fig. 5 : n-Haptane mole fraction for emulsions with water contents of 25% and 35% in a surrogate fuel of 70% n-Heptane and 30% Toluene.

Fig. 6 shows the effect of water content on CO, where CO and UHC are produced as a result of incomplete combustion. At high temperatures with more sufficient time, these two products further oxidize and form carbon dioxide and water.

As shown in Fig. 6, the final CO concentration increases with increasing water content in the emulsion. Water reduces the temperature inside the combustion chamber to a level where CO oxidation is inhibited. The reaction rates of CO with O, O_2 and OH decrease with decreasing temperature. Therefore the production rate of CO is increased. CO production rates for the two water contents are shown in Fig. 7 where the peak CO production rate increases as the water content increases.

The increase of CO level with increasing water content was experimentally validated by several researchers [13].

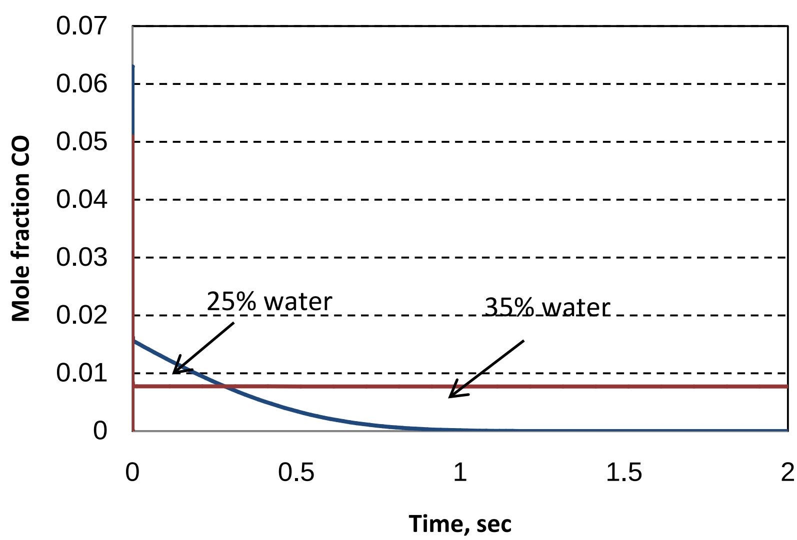

Fig. 6 : CO mole fraction for 25% and 35% water content in emulsion with 70% n-Heptane and 30% Toluene.

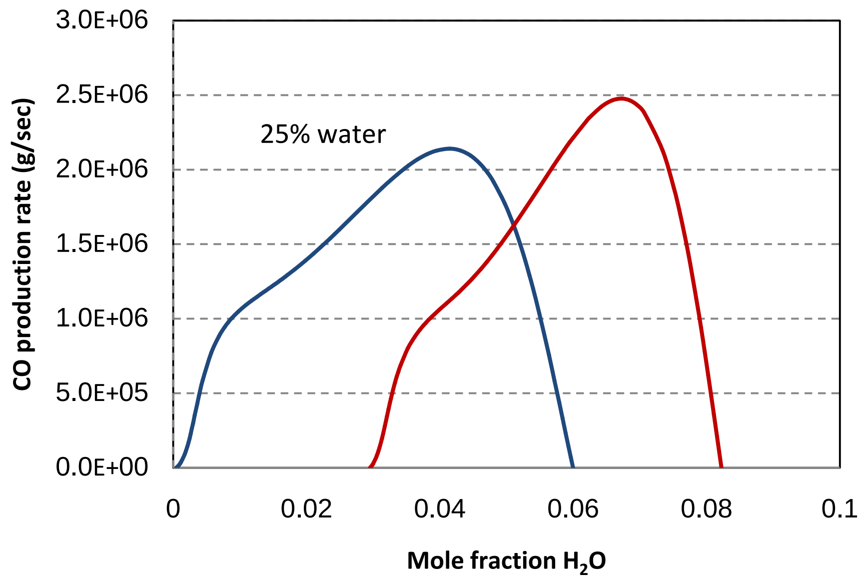

Fig. 7 : CO production rate (g/sec) for 25% and 35% water content in emulsion with 70% n-Heptane and 30% Toluene.

Fig. 8 shows the effect of water content on the UHC and VOC. As shown in the figure the amount of UHC increases as the water content increases. This result agrees with the findings of Milton and Carter, who showed for tests simulating a typical city driving cycle that UHC tend to increase by water injection [14], and with the findings of Prakash et al. [16].

UHC emissions are direct result of incomplete combustion of fuel. As water content in the emulsion increases, longer ignition delay and lower combustion temperature are usually experienced which may lead to the emission of more partially oxidized hydrocarbons [14, 16].

Therefore, while benefits to several pollutant emissions occur as a result of water addition to the fuel, these may be offset by the increase in CO and UHC emissions. However, researchers used emulsions of water with heavy oil [13] and biodiesel [2] reported a decrease in UHC emissions with increasing water content and thus the effect of water on UHC emissions needs further thorough investigation. Fig. 8 also shows the effect of water content on VOC emissions which like the UHC, increase with increasing water content. VOC are typically not acutely toxic, but instead may have compounding long-term health effects.

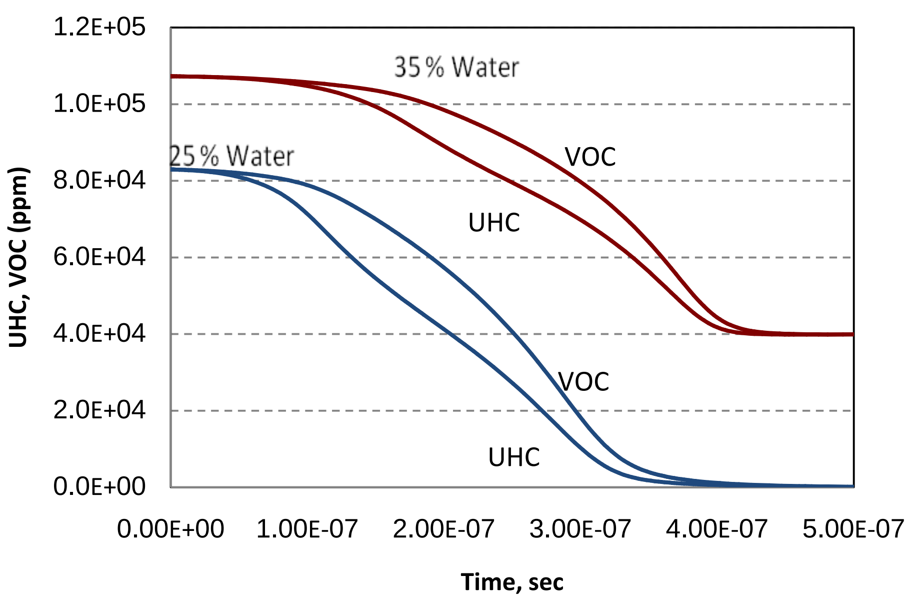

Fig. 8 : UHC and VOC for 25% and 35% water content in emulsion with 70% n-Heptane and 30% Toluene.

The effect of water content on propargyl C_3H_3 formation is shown in Fig. 9. C_3H_3 concentration decreases with increasing water content. C_3H_3 is a major precursor to form Polycyclic Aromatic Hydrocarbons PAH as two molecules of C_3H_3 can combine together to form Benzene ring C_6H_6. For low water contents, El-Sinawi [15] found that the formation of C_3H_3 decreases with increasing water content up to 5% then it increases when higher amounts of water were added with surrogate fuel composed of 80% n-Heptane and 20% Toluene.

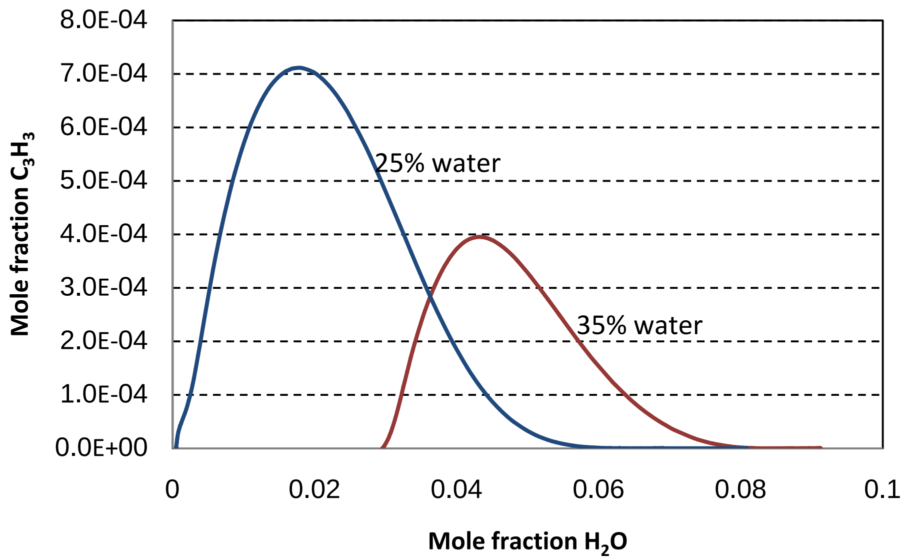

Fig. 9 : C_3H_3 mole fraction for 25% and 35% water contents in emulsion with 70% n-Heptane and 30% Toluene.

The effect of water content on Benzene formation is shown in Fig. 10. Benzene concentration decreases with increasing water content. Benzene can combine with Toluene and therefore has an important role in PAH and soot formation [4].

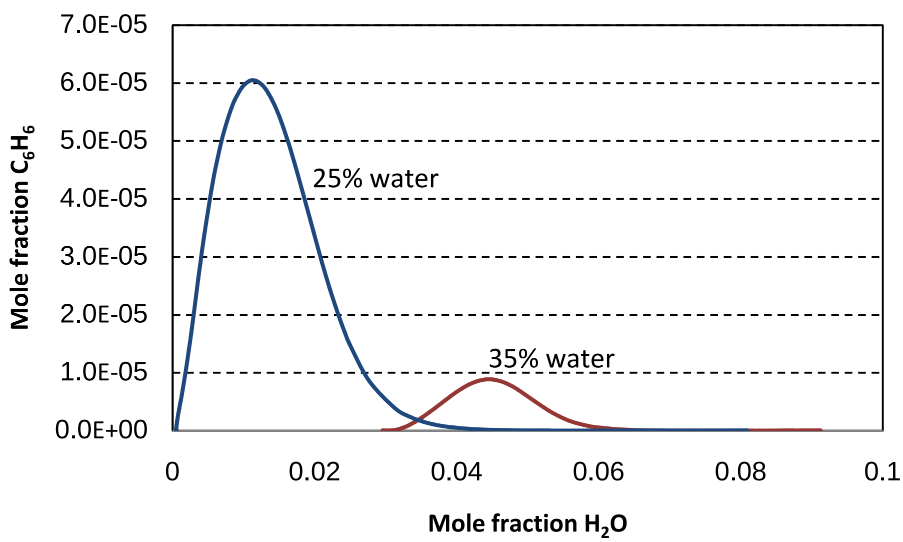

Fig. 10 : Benzene mole fraction for 25% and 35% water contents in emulsion with 70% n-Heptane and 30% Toluene.

Fig. 11 shows the effect of water content on the concentration of fulvene, which is a toxic compound. Increasing water content decreases fulvene emissions.

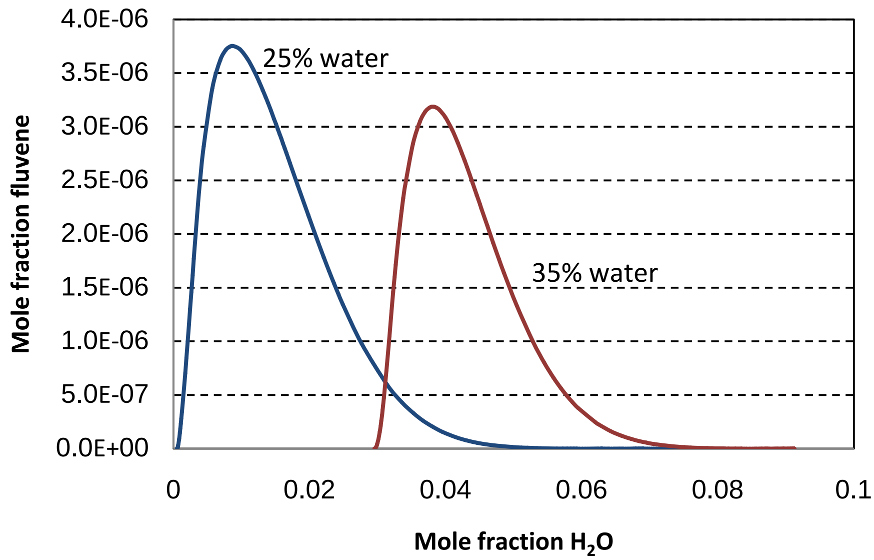

Fig. 11 : Fulvene mole fraction for 25% and 35% water contents in emulsion with 70% n-Heptane and 30% Toluene.

The concentration of nC_3H_7 group is shown in Fig. 12. nC_3H_7 can lead to the formation of formaldehyde which is very toxic and corrosive. The concentration of nC_3H_7 decreases as water content in the emulsion increases.

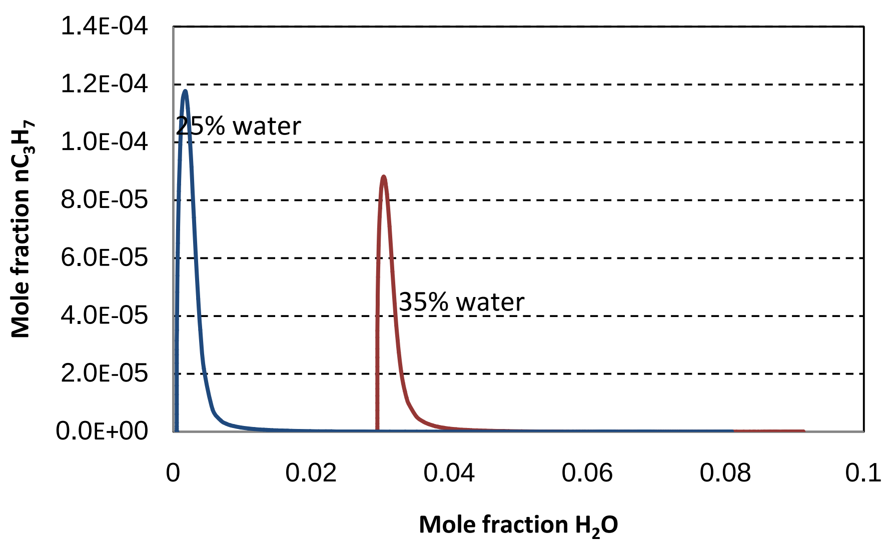

Fig. 12 : nC_3H_7 mole fraction for 25% and 35% water content in emulsion with 70% n-Heptane and 30% Toluene.

IV. Conclusions

The effect of adding a relatively high percentage of water to surrogate fuel composed of 70% n-Heptane and 30% Toluene on the formation of pollutants was discussed. The use of water-in-fuel emulsion is an effective technique to reduce pollutant emissions from surrogate fuel even at relatively high water contents of 25% and 35%. It was found that as water content increases the reduction of the emissions studied increases and the fuel consumption slightly decreases. However, the tradeoff with CO and UHC emissions was maintained.

V. Abbreviations

CO	Carbon Monoxide
CO_2	Carbon Dioxide
CO_x	Carbon Oxides
NO	Nitrogen Monoxide
NO_2	Nitrogen Dioxide
NO_x	Nitrogen Oxides
PAH	Polycyclic Aromatic Hydrocarbons
UHC	Unburned Hydrocarbons
VOC	Volatile Organic Compounds

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