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NUMERICAL CHARACTERIZATION OF DIFFERENT N-DECANE-ETHANOL BLENDS COMBUSTION

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Abstract. *Research and investments in renewable energy are important to reduce oil dependence, to improve energetic safety and to reduce environmental and public health damages caused by combustion emissions. Currently, diesel is the most popular fossil fuel in several countries, including Brazil, Paraguay and France. Sugar cane ethanol is widely used as fuel in Brazil, but only in Otto cycle engines. Nevertheless there are diverse researches revealing that it can be added to diesel and reduce particulate matter emissions of Diesel cycle engines among other advantages. Due to diesel chemical complexity, n-decane is usually used as a diesel simplified surrogate fuel. The objective of this work is to unveil the effects of ethanol addition in n-decane combustion. REGATH package was used in numerical simulation. A new chemical scheme was developed putting together two already validated chemical schemes simulating 1D premixed laminar flames. This scheme allows prediction of several combustion characteristics. Blends ranging from 5% to 30% ethanol (mol) were simulated with equivalence ratios ranging from 0.8 to 1.4. For each blend, flame speed, flame thickness, maximum temperature and CO and CO_2 emissions were obtained. Blend's results were similar to n-decane results, unveiling that the studied combustion properties did not change for ethanol proportions added.*

Keywords: *n-decane-ethanol blend, combustion, flame speed, flame thickness, flame temperature*

1. INTRODUCTION

Petroleum and oil products were responsible for 39,3% of Brazilian domestic energy supply in 2013. 118 117 000 m^3 of petroleum were consumed. Almost half of it was transformed into diesel: total domestic consumption of diesel was 57 783 000 m^3, of which 75.8% were used by transport on highways. Diesel is also used in railroads and waterways. Beyond transports, other activities use this fuel: agriculture and livestock, and several industries - from chemistry to foods and beverages (Empresa de Pesquisa Energética, 2014).

The development of a chemical scheme that properly describes the combustion process of commercial diesel would be very complex, because this fuel consists in hundreds of chemical species. Thence a surrogate fuel is usually studied instead. A surrogate is a simpler representation of a composite fuel, consisting in a small number of pure compounds that have combustion characteristics similar to the target real fuel (Chang *et al.*, 2013; Farrell *et al.*, 2007). N-decane has been used as major component of diesel surrogates in several studies (Lemaire *et al.*, 2009, 2013; Weber *et al.*, 2007; Wang *et al.*, 2010). In this paper, a chemical scheme of pure n-decane was put together with an ethanol scheme in order to analyze it's behaviour.

There are two main advantages in replacing fossil fuels by renewable fuels: energy security, since there are limited petroleum reserves and they are mainly concentrated in few countries; and emissions control. Ethanol is an interesting alternative fuel because it is oxygenated, so it cans reduce particulate matter emissions in compression-ignition engines (Agarwal, 2007). Furthermore, it is widely available and it has an attractive price in the Brazilian market.

Ethanol and diesel have different physicochemical properties that need to be considered when ethanol is intended to be used in compression-ignition engines. Main properties to be evaluated are stability, viscosity, lubrication, energy content and cetane number (Hansen *et al.*, 2005). There are technical solutions according to each utilization: if it is intended to use 100% Ethanol in compression-ignition engines, it is necessary to use additives to improve compression ratio and injection flow mass (Britto and Martins, 2015) and to verify material compatibility. Most researches focus ethanol-diesel blends with less than 10% of ethanol (volumetric) (De Caro *et al.*, 2001; Sayin, 2010; Huang *et al.*, 2009; Di *et al.*, 2009; Rakopoulos *et al.*, 2008; Putrasari *et al.*, 2013). That is the range analyzed in this study in n-decane-ethanol blends.

There are few study in basic characterization of diesel-ethanol blends combustion (Zhu *et al.*, 2015; Moon *et al.*, 2013). A detailed kinetic mechanism for turbulent combustion would be stiff and have a high computational cost. So a laminar flame is studied, and it's mechanism must be known in order to study turbulent flame mechanism. Flame speed is an important characteristic because flame shape, blowoff, flashback and other important flame-stability characteristics depend on it. Flame thickness is the thin region were the reaction occurs (Turns *et al.*, 1996). It is also important to know maximum combustion temperature in order to define materials to be used in engines (Agarwal, 2007).

The aim of this study is to model a chemical scheme for n-decane-ethanol blends and to compare flame speed, flame thickness, maximum temperature and emissions for different blends proportions and equivalence ratios.

2. NUMERICAL SIMULATION

A combustion problem can be formulated using equations of conservation of mass, momentum and energy, thermodynamic relations, and chemical kinetics mechanisms: elementary chemical reactions and it's respective reaction rates. A chemical kinetic mechanism describes at a molecular level how, through intermediate species, reactants are transformed in products. It is usually used to predict cool flame characteristics, soot and pollution formation, knocking limits, ignition behavior and energy release rate (Westbrook and Dryer, 1984; Alviso, 2013).

2.1 Chemical Schemes

The objective of the present work was to develop a new chemical scheme putting together the n-decane model described by Marchal et al., 2009 and the ethanol scheme described by Marinov, 1999.

The n-decane scheme used (Marchal *et al.*, 2009) was developed using literature data and new detailed reaction mechanisms. It can be used to describe m n-heptane, iso-octane, n-decane and kerosene combustion. The scheme has 154 species and 850 reactions.

The ethanol scheme used (Marinov, 1999) was assembled using previously developed reaction sub-mechanisms for hydrogen, methane, ethane, propane and ethylene. It consists of 57 species and 387 reactions.

To develop the new scheme, Marchal et al (2009) scheme and Marinov (1999) scheme were compared to find out which chemical reactions they had in common. Then, they both were altered in the same way: the basic skeleton of each scheme was maintained, and the reactions that were not common to both schemes were added to the one that did not have them. The result was two different new chemical schemes, with the same 171 species and 1010 reactions; but with different rate coefficients because each skeleton used had it's own coefficients values. Both schemes were used to simulate methane, ethanol and n-decane and results obtained were compared to literature in order to find out which one better describes the combustion of these fuels. The chosen scheme was used to simulate n-decane-ethanol blends.

2.2 Simulation Conditions

Flame simulations were performed using REGATH package, developed at EM2C laboratory (Candel S, 2011). A 1D premixed flame model were used. Equations were used as described at Aguerre (1994). Combustion was assumed to start at initial temperature of 400K, and at atmospheric pressure (1 bar). Equivalence ratio was varied from 0.8 to 1.4. Combustion of pure ethanol (E100) and pure n-decane were simulated using the new chemical scheme developed, in order to validate it comparing results with literature experimental and numerical data. After that, blends combustion were simulated. The n-decane-ethanol blends molar proportions chosen were: 5% Ethanol- 95% N-decane (E05), 10 % Ethanol - 90% N-decane (E10), 15% Ethanol - 85% N-decane (E15), 20% Ethanol - 80% N-decane (E20), 25% Ethanol - 75% N-decane (E25) and 30% Ethanol - 70% N-decane (E30). Table 1 presents volumetric ethanol equivalence for these blends. Flame speed, flame thickness, maximum flame temperature and CO and CO_2 emissions were compared.

3. RESULTS

It was simulated a 2000mm tube. Scale ranged from -1000mm to 1000mm. Combustion starts at 0mm. Figures 1 and 2 emphasize where combustion occurs and values change.

Figure 1 presents a comparison between flame temperature profiles simulated by the new scheme and the one described by Marchal et al (2009) with equivalence ratio = 1.0. Maximum temperature found by the new scheme was 3.4% higger than the one found by Marchal et al (2009) scheme. This difference is small.

Table 1 - Volumetric ethanol percentages in simulated blends

Blend (molar)	% of ethanol (volume)
E05	1.34
E10	2.78
E15	4.35
E20	6.05
E25	7.91
E30	9.94

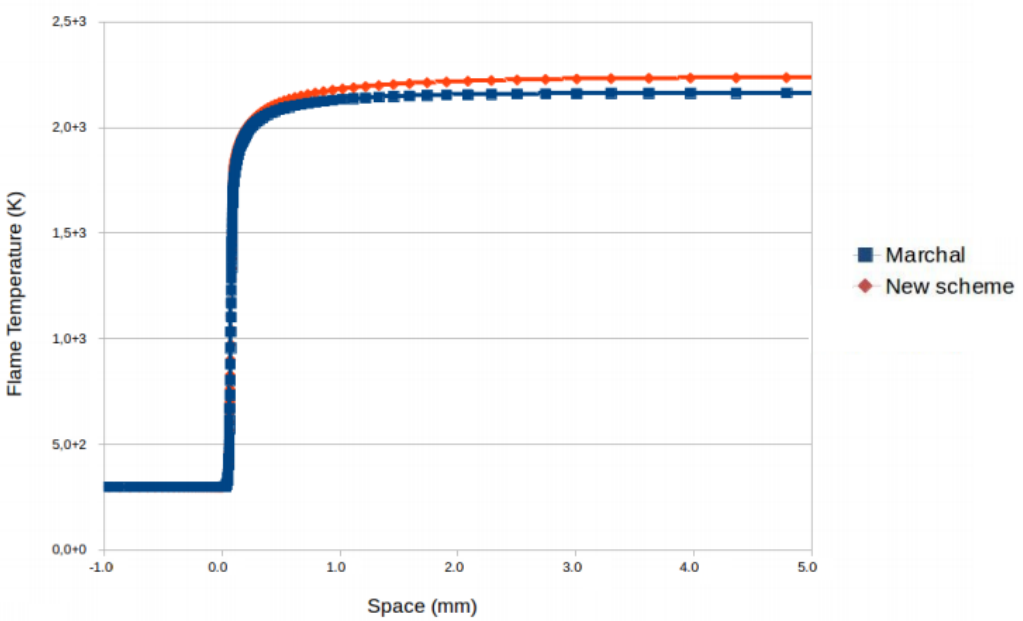

Figure 1: Comparison between temperature profiles of n-decane simulated by the new scheme and the scheme presented by Marchal et al (2009), with equivalence ratio= 1.0

Figure 2 presents a comparison between consume of n-decane mass fraction simulated by the new scheme and the Marchal et al (2009) scheme with equivalence ratio = 1.0. Again, results found were very similar, revealing that the new scheme is reliable

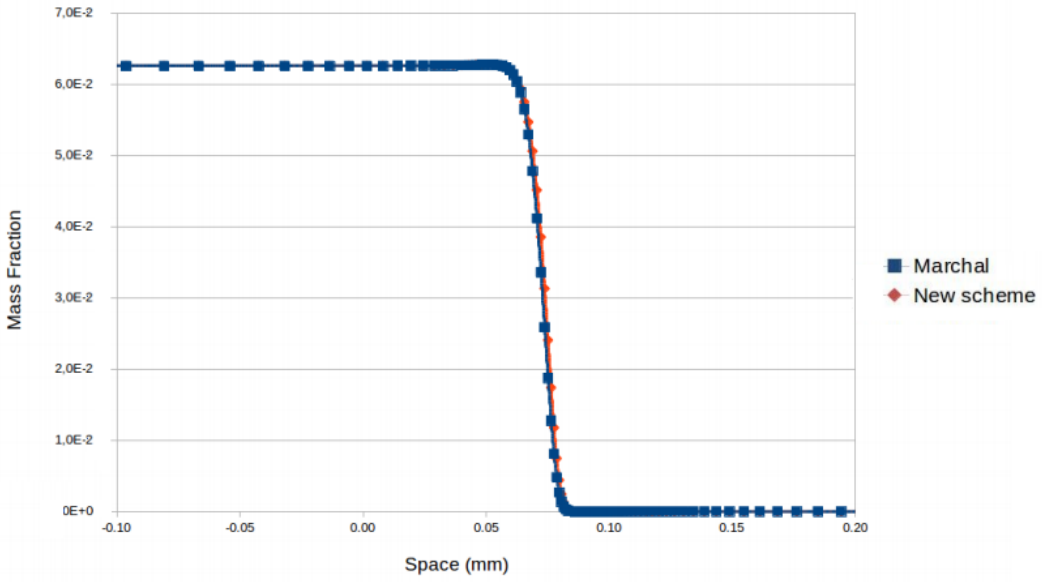

Figure 2: Comparison between n-decane mass fraction profiles simulated by the new scheme and the scheme presented by Marchal et al (2009), with equivalence ratio = 1.0

Figure 3 presents a comparison between n-decane flame speeds for different equivalence ratios using the reference chemical scheme; the chemical scheme described by Chang et al., 2013 ; the developed scheme and experimental data found in the literature: Munzar et al., 2013; Comandini et al., 2015; Kim et al., 2013; Ji et al., 2010; Kumar and Sung, 2007; Singh et al., 2011; Hui and Sung, 2013. It reveals that the new scheme developed approaches significantly of the experimental data. In order to quantify this proximity, an average of literature experimental data was taken and compared with the numerical simulations avaiable. The new model flame speed was closer to this average than the other models when equivalence ratio is equal or higger than 1.0. Since the literature presents some different experimental conditions, this new model still needs to be experimentally validate. Nevertheless, this comparison suggests that the model is appropriated.

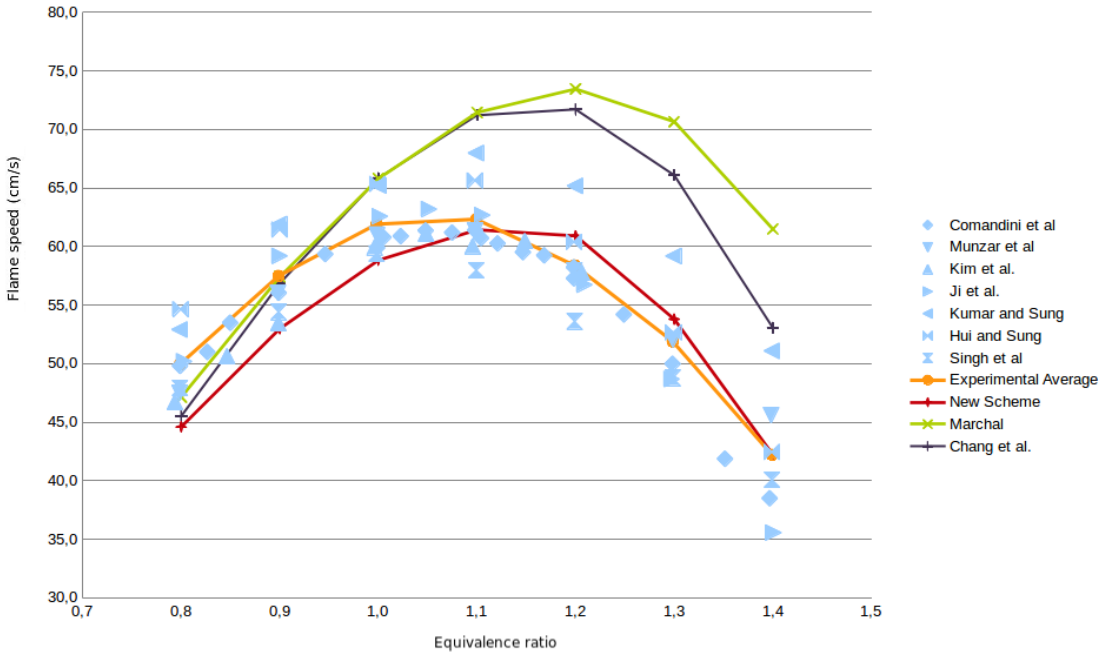

Figure 3: Pure n-decane flame speed found by the chemical scheme developed and experimental and numerical data available in the literature for different equivalence ratios

Figure 4 compares flame speed of pure ethanol, pure n-decane and different n-decane-ethanol blends for different equivalence ratios. Values found for all blends were very similar. Small ethanol proportions slightly decrease flame velocities for equivalence ratios stoichiometric or higger, but the values did not differ significantly from n-decane flame speeds. The main aspects that affect flame speed are gas temperature, pressure, equivalence ratio and fuel type (Turns *et al.*, 1996). In this simulation, the three first parameters were maintained constant, so the fuel type would be responsible for differences observed. Ethanol flame speed was simulate as well. For each equivalence ratio, it is about 20 cm/s faster then blends velocities.

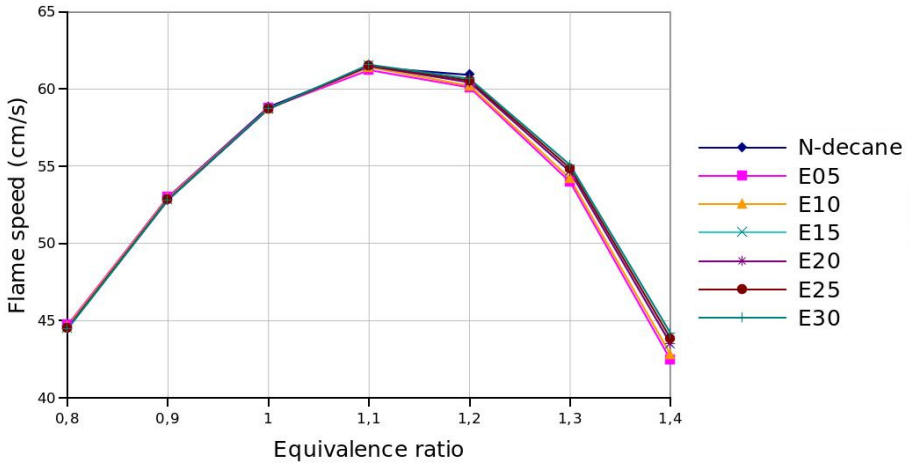

Figure 4: Flame Speed as a function of equivalence ratio for different n-decane-ethanol blends

Figure 5 compares flame thickness of pure ethanol, pure n-decane and different n-decane-ethanol blends combustion for different equivalence ratios. Flame thicknesses were close between blends and n-decane, and not so far of ethanol.

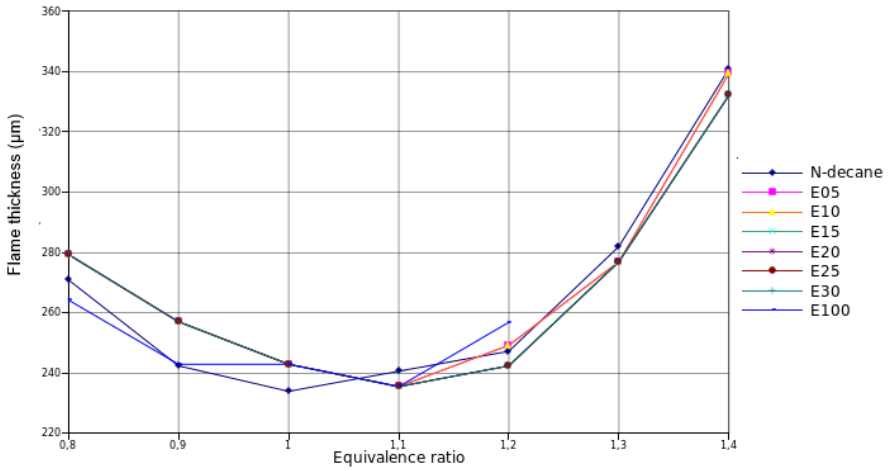

Figure 5: Flame Thickness versus Equivalence Ratio for different n-decane-ethanol blends

Figure 6 compares maximum temperature of different n-decane-ethanol blends at different equivalence ratios. Maximum temperatures were the same between blends and really close of n-decane maximum temperatures. This combustion characteristic depends on fuel thermodynamic properties (Turns *et al.*, 1996).

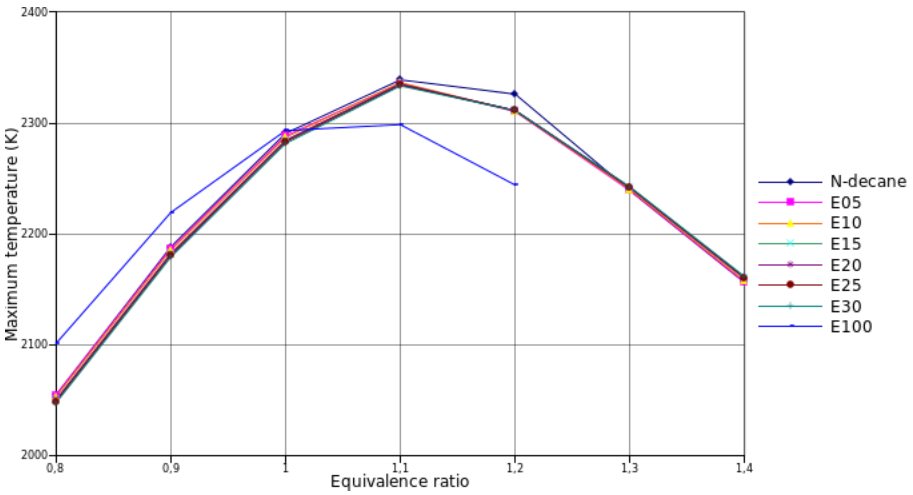

Figure 6: Maximum Temperature versus Equivalence Ratio for different n-decane-ethanol blends

Figure 7 compares CO emissions of different n-decane-ethanol blends at different equivalence ratios. Ethanol emissions are almost zero, and that is one of the reasons why this bio-fuel is interesting for the environment. Blends emissions were close to n-decane emissions and increase when equivalence ratio is increased.

Figure 8 compares CO_2 emissions of different n-decane-ethanol blends at different equivalence ratios. Different from that observed for CO, CO_2 ethanol emissions were comparable to n-decane and blends emissions, being igger then them in most simulated equivalence ratios. Ethanol is obtained from vegetables that use CO_2 to grow, so that is why it is considered carbon clean. In the other hand, it is important to consider that ethanol has it's own possible dangerous emissions, such as acetaldehyde. Those emissions still need to be properly studied and regulated (Poulopoulos *et al.*, 2001).

Experimental data need to be collected to validate the model and to evaluate other important combustion characteristics and emissions.

4. CONCLUSIONS

A new chemical scheme that describes n-decane-ethanol blends combustion was developed. The new scheme was able to describe experimental data from literature better then others preexisting tested schemes. Blends up to 30% ethanol in mol were analyzed, and flame velocities, flame thickness, maximum flame temperature and CO and CO_2 emissions did

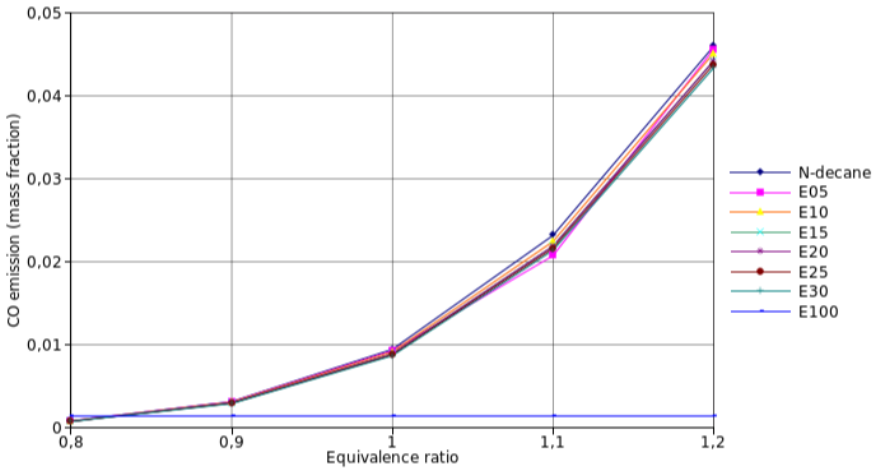

Figure 7: Maximum CO emission versus Equivalence Ratio for different n-decane-ethanol blends

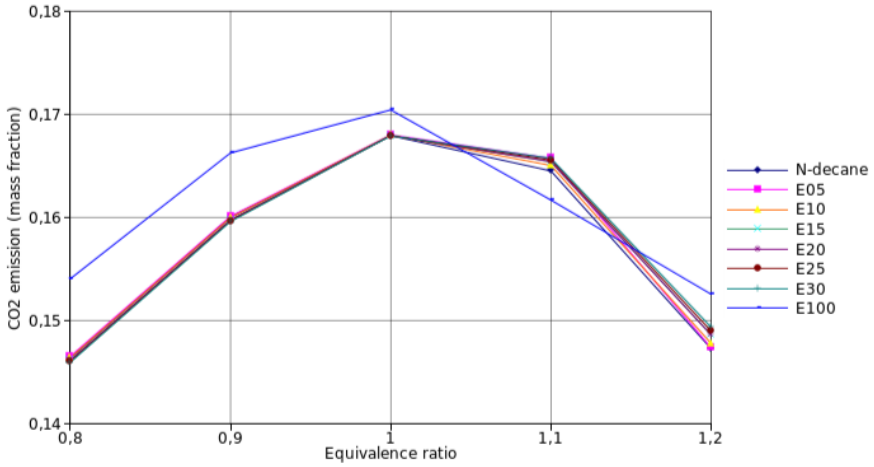

Figure 8: Maximum CO_2 emission versus Equivalence Ratio for different n-decane-ethanol blends

not differ significantly from 100% n-decane. Experimental data need to be collected to validate the model.

5. ACKNOWLEDGEMENTS

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