# NUMERICAL SIMULATION OF THE PERFORMANCE PARAMETERS OF AN OTTO ENGINE RUNNING ON ETHANOL AT DIFFERENT PERCENTAGES OF HYDRATION

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***Abstract.*** *Ethanol is an environment friendly fuel as on its life cycle the carbon dioxide generated during production and combustion is absorbed by the crops during photosynthesis in their growth process. Broader inflammability limits, higher knock resistance and higher heat of vaporization, when compared to gasoline, are some characteristics to be explored in internal combustion engines aiming at achieving higher efficiency. Recent researches show that it is possible to run engines with high water-in-ethanol content and achieve higher efficiency levels than those achieved with conventional Otto engines. The water addition reduces the laminar flame velocity and end gas temperature. Studies also show that energy consumption increases exponentially to achieve ethanol-in-water levels above 70%. In this scenario, this paper proposes a sensibility study of indicated performance values and combustion parameters of a 0,668-L Otto cycle engine running on ethanol at different percentages of hydration through one-dimensional commercial code. For water-in-ethanol content from 0% to 40% and different combustion durations, indicated parameters of MEP, volumetric efficiency, thermal efficiencie and knock related parameters are compared. It is found that with water addition volumetric efficiency is enhanced, while different combustion durations directly affect heat transfer and engine thermal efficiency.*

**Keywords:** *hydrous ethanol, internal combustion engine, ethanol in water.*

## 1. INTRODUCTION

To obtain clean and renewable energy sources is a challenge for the humanity. With the increase in energy requirements and the rising cost of oil, the concept of “green energy” is standing out. This source of energy should not contribute to greenhouse effect and must be accessible with competitive prices compared to fossil fuels. For ethanol, total release of CO2 on the production and burn stage is balanced by absorbed $CO_2$ in the photosynthesis process from crops it is obtained, this way contributing to reduce the greenhouse effect.

Bioethanol production methods are basically constituted of feedstock formation, mashing and cooking, fermentation and dehydration. Before the beginning of distillation phase, after fermentation, ethanol-in-water content varies from 6%to 12% (Ladisch and Dyck, 1979). Distillation can be performed to obtain 95,5% of ethanol-in-water content, the azeotropic limit of the mixture and the production cost is exponentially enhanced to dehydrate from over 70% of purity (Flowers et al., 2007). To obtain anhydrous ethanol dehydration through adsorption in vapour phase with molecular sieves can be done at high energy cost. Figure 1 shows the net energy gain considering sugarcane anhydrous ethanol (a) and 20% water-in-ethanol (b).

Therefore, the use of hydrous ethanol can be more economically attractive than anhydrous ethanol and more competitive with fossil fuels (Cardona and Sánchez, 2007). In this scenario, hydrous ethanol stands as a great opportunity to be explored in internal combustion engines.

Studies conducted on Otto engines running with high water-in-ethanol content and gasoline blends show that there is a limit of gasoline in the mixture due to miscibility issues (Rajan and Saniee, 1983; Nguyen and Wu, 2009). It is also shown lower unburned HC and NO emissions compared to pure gasoline. In other way, with low water-in-ethanol content (4% to 7% of water) and gasoline blends NO emission is highly dependent on the fuel to air ratios and operation conditions (Turner et al., 2007; Machado et al., 2012). Subramanian et al. (2006) found that water injection is very effective to control NO emission and hydrogen knocking due to in cylinder peak temperature reduction. The use of water-gasoline emulsions on SI engines increases engine thermal efficiency but decreases the lean limit of the mixture due to charge dillution (Nguyen and Wu, 2009). Özcan and Söylemez (2005) studied manifold water injection on a SI engine running with liquefied petroleum gas. Again, water reduced charge and exhaust gas temperatures, consequently reducing NO emissions, burning rate is also reduced and engine thermal efficiency increases. For the higher auto-ignition endurance of ethanol compared to gasoline, higher compression ratios can be achieved enhancing thermal efficiency (Turner et al., 2007; Giroldo et al., 2005).

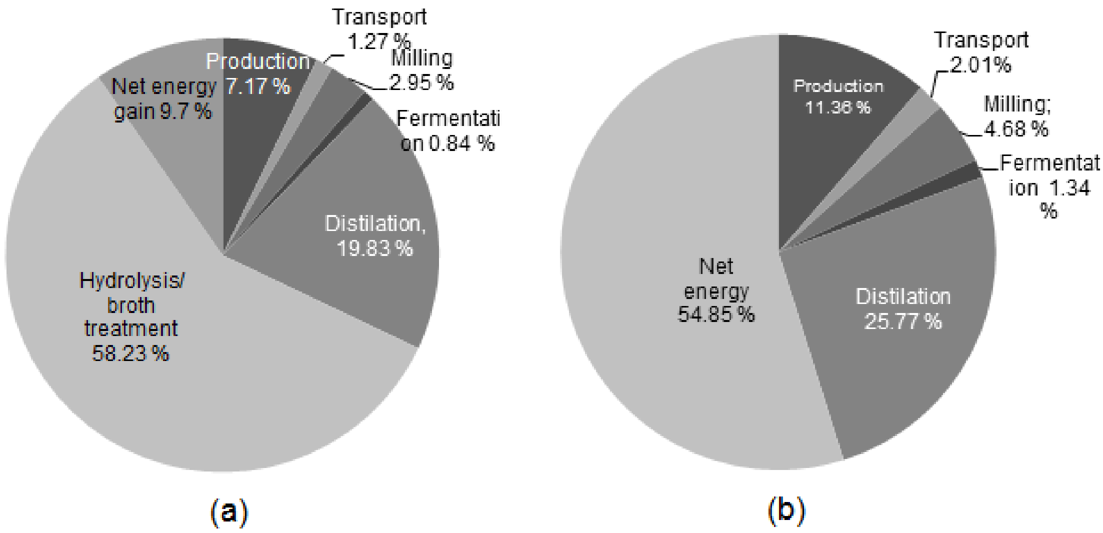


Figure 1 - Net energy balance in (a) Sugar cane anhydrous ethanol, (b) 20% of hydration. The figure indicates energy consumption in all stages of the Sugarcane ethanol production as percent of the heating values in $MJ.L^{-1}$ (Salla et al., 2009)

This characteristic makes ethanol an anti-knock additive to gasoline (Bromberg and Bloomberg, 2009). Recent studies shown that HCCI engines can operate with water-in-ethanol percentages up to 40%, achieving brake engine efficiencies around 40% (Flowers et al., 2007; Mack et al., 2009; Boretti, 2012).

Knowing that premixed laminar flame speed of fuels is reduced by water addition (Mazas et al., 2011), the same is expected to combustion duration on internal combustion engines (Parag, S. and Raghavan, 2009). Therefore this paper aims to develop a sensibility study of the indicated parameters of efficiency and combustion of an Otto engine running with hydrated ethanol with water content from 0% to 45% through numerical simulation in GT-Power commercial code.

## 2. ENGINE SIMULATION

Engine simulation has been performed on GT-Power, one of the market leaders in one-dimensional engine gas dynamics simulation. It has been largely used by engine manufacturers worldwide to provide fast and cheap results compared to experimental analysis (Neumann et al., 2007; Birckett and Keidel, 2011).In Bos (2007), a GT-Power model validation is well explained. Figure 2 shows simulation results compared to experimental data to mass flow rate and in-cylinder pressure for a motored condition on an experimental turbocharged engine showing good agreement. Also, GT-Power allows the evaluation of operation parameters without the computational and time costs of a 3D finite volume codes simulation.

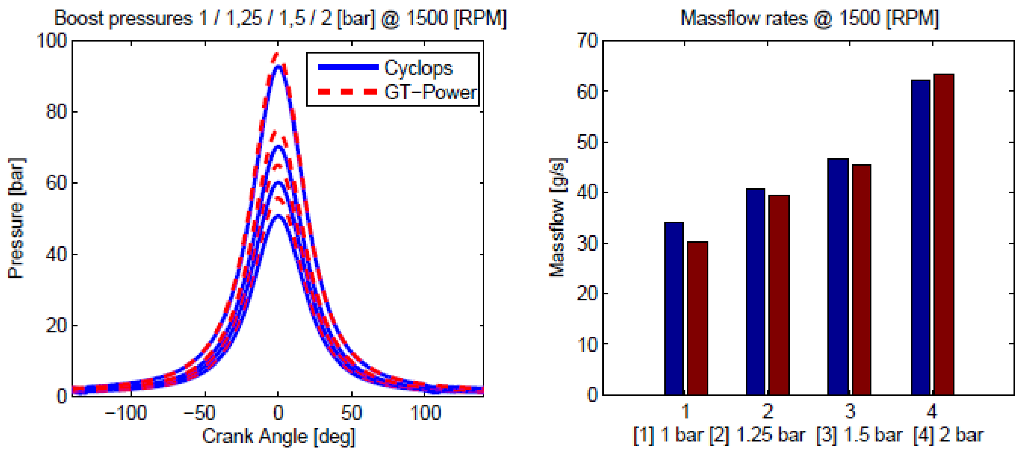


Figure 2 – Comparison of GT-Power simulation to experimental data

The engine characteristics and a comparison between some ethanol and gasoline proprieties are shown in Tab. 1 and Tab. 2 respectively. The reference fuel ethanol ($C_2H_6O$) and water (H2O) are injected at the entrance of the intake port.

Table 1. Engine characteristics.

| Strokes | Bore (mm) | Stroke (mm) | Conecting rod Length (mm) | Compression ratio | Displaced volume (dm³) |
|---|---|---|---|---|---|
| 4 | 90 | 105 | 160 | 14 | 0.668 |

Table 2. Fuel proprieties.

| Fuel | Density¹* (kg/m³ @ 0 °C, 1 atm) | Heat of Vaporization* (kJ/kg) | Stoichiometric Air/Fuel Ratio** | RON** |
|---|---|---|---|---|
| Ethanol | 0.785 | 924 | 9 | 107 |
| Gasoline | 0.75 | 350 | 14.6 | 95 |

*From GT-Power database
**From Heyood 1988

Combustion is described as an imposed Wiebe function, as per equation (5) (GT-Power Reference Manual, 2010) to model heat release rate in a two zone model, whichseparates the combustion chamber in burned and unburned zones, assuming homogeneous proprieties for each zone. The cumulative burn rate is calculated as normalized to 1.0. The Wiebe exponent parameter describes the function shape andthe heat release distribution through the whole combustion duration. It is known that high in-cylinder flow motion speeds up combustion and water addition to fuels decreases combustion speed due to laminar flame speed reduction. Slow reaction in the initial phase and explosion like combustion profiles could be modelled through the “E” parameter. Theliterature, however, does not provide enough information about the Wiebe function shape parameter as a function of variouswater-in-ethanol contents. Thus, for comparison purposes, parameter “E” value is chosen following a general literature example, Heywood (pg. 390, 1988), the same value used as default in GT-Power model.

As no burn rate and combustion profiles for ethanol with increased water content inspark ignited engines are found in literature, this study will evaluate the influence of water-in-ethanol content – from 0% to 40% – in spark ignited engine performance through several case studies where combustion duration varies from 30º to 70º crank angle. MBT (minimum spark advance for maximum brake torque) is achieved varying the Anchor Angle in each case study.

$$BMC = -\ln(1 - BM) \quad (1)$$

$$BSC = -\ln(1 - BM) \quad (2)$$

$$BEC = -\ln(1 - BM) \quad (3)$$

$$WC = \left[\frac{D}{BEC^{\left(\frac{1}{E+1}\right)} - BSC^{\left(\frac{1}{E+1}\right)}}\right]^{-(E+1)} \quad (4)$$

$$SOC = AA - \frac{D.BMC^{\left(\frac{1}{E+1}\right)}}{BEC^{\left(\frac{1}{E+1}\right)} - BSC^{\left(\frac{1}{E+1}\right)}} \quad (5)$$

$$Combustion(\theta) = CE\left[1 - e^{-(WC)(\theta - SOC)^{E+1}}\right] \quad (6)$$

Where:
AA = Anchor Angle (Varied for MBT achievement)
D = Duration (Varied from 30º to 70º)
E = Wiebe Exponent (input used: 2.0)
CE = Combustion Efficiency (input used: 1.0)
BM = Burned Fuel Percentage at Anchor Angle (input used 50%)
BMC = Burned Midpoint Constant
BS = Burned Fuel Percentage at Duration Start (input used 10%)
BSC = Burned Start Constant
BE = Burned Fuel Percentage at Duration End (input used 90%)
BEC = Burned End Constant
SOC = Start of Combustion (Calculated for each case)

WC = Wiebe Constant (Calculated for each case)
θ = Instantaneous Crank Angle

A Woschni correlation (Heywood, pg. 679, 1988) is used to predict in-cylinder heat transfer. For this paper, it is assumed that the engine is knock-free at full load when running on 100% ethanol. This way, the end gas temperature is evaluated to determine the possible occurrence of knock with water-in-ethanol content increase.

For combustion durations of 30°, 40°, 50°, 60° and 70° crack angle and ethanol-in-water content varying from 0%-100% to 40%-60%, equivalence ratio of 1 (stoichiometric combustion) is simulated while water-in-ethanol content varies for different combustion durations;

## 3. RESULTS

Simulation results were achieved after full engine modelling for combustion durations varying from 30° to 70° crank angle with water-in-ethanol content varying from 0% to 40%. In cylinder ethanol to air ratio was monitored to ensure stoichiometric conditions for all simulations. For each combustion duration and water-in-ethanol mixture content MBT was achieved varying the Wiebe Anchor Angle.

Figure 3 shows volumetric efficiency behaviour of the engine for different water-in-ethanol contents. As expected, simulations shown that combustion duration have very little impact in the volumetric efficiency. Volumetric efficiency is highly dependent on manifold geometry, inlet fluid state – mainly temperature and pressure – and engine speed. As all case studies were simulated for the same inlet manifold geometry in the same engine speed of 1800 RPM, the increase in volumetric efficiency is attributed to the high heat o vaporization of water, which increases fluid density allowing more charge to be inducted in the cylinder at each cycle.

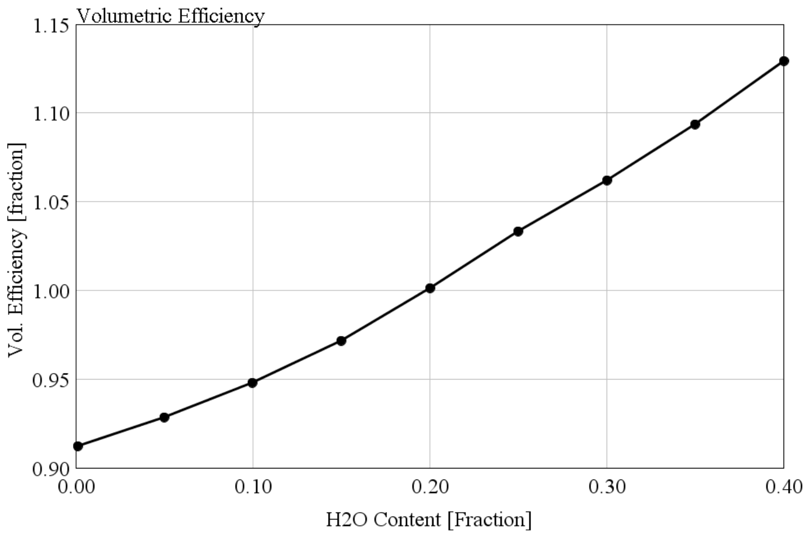


Figure 3 – Volumetric efficiency

It can be seen from Figure 4 that faster combustion increases IMEP due to better energy conversion from combustion to piston work. Even though MBT is achieved for each combustion duration and water-in-ethanol content, it is clear that as combustion duration increases, more energy is released away from the optimum piston position, i.e., with bad phasing. Also, for all combustion durations, as water-in-ethanol content is increased, IMEP becomes higher. It can be explained due to the fact that combustion efficiency is kept constant in all cases and all fuel energy is always released with stoichiometric combustion added to the fact that more charge can be inducted in the cylinder at each cycle. Also, as water content increases, its volume occupies more space in the cylinder, increasing the effective compression ratio of the charge.

Figure 5 shows that the percentage of total fuel energy transferred to in-cylinder walls reduces while water-in-ethanol content increases. Meanwhile, total fuel energy leaving the cylinder in exhaust process is increased by the same amount, as it is shown in figure 6. The in-cylinder gas to wall heat transfer has a complex behaviour when looking at combustion duration and its effect is highly correlated to mean piston speed and convection heat transfer coefficient, which is calculated through the classic Woschni correlation (Heywood, pg. 679, 1988). A detailed analysis of this parameter is out of the scope of this work and should be more detailed studied in future works.

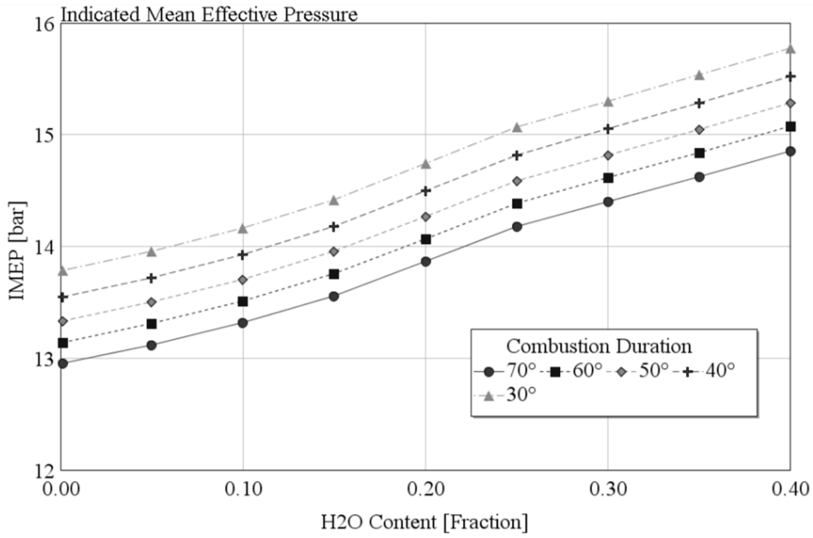


Figure 4 – Indicated Mean Effective Pressure

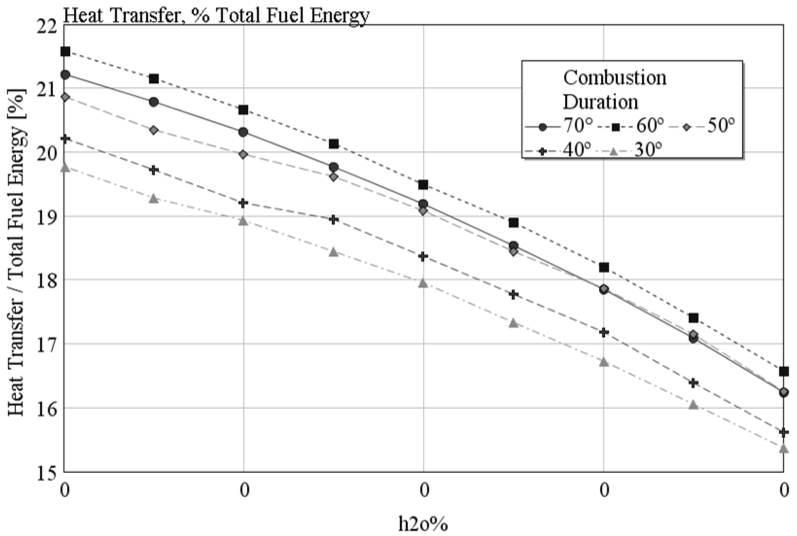


Figure 5 – Total fuel energy percentage lost due to in-cylinder gas to wall heat transfer

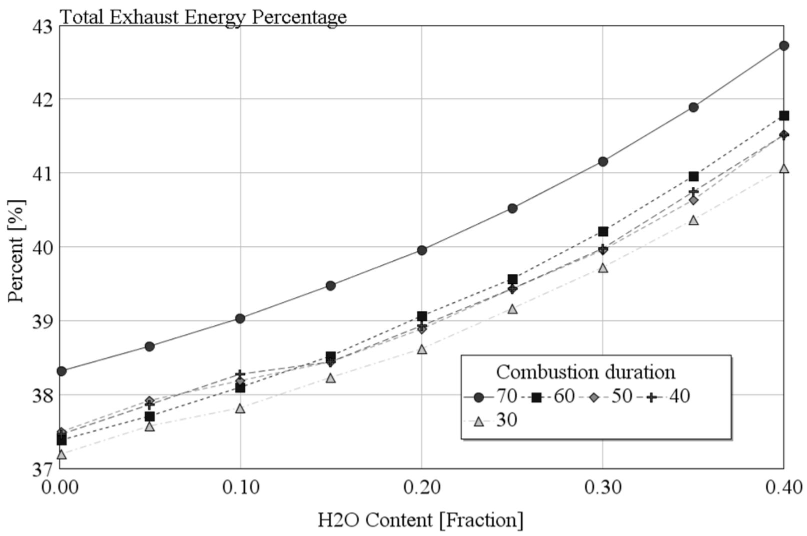


Figure 6 – Total fuel energy lost in exhaust gas-exchange process

Finally, the indicated thermal efficiency slightly increases as water-in-ethanol content increases as shown in Figure 7.

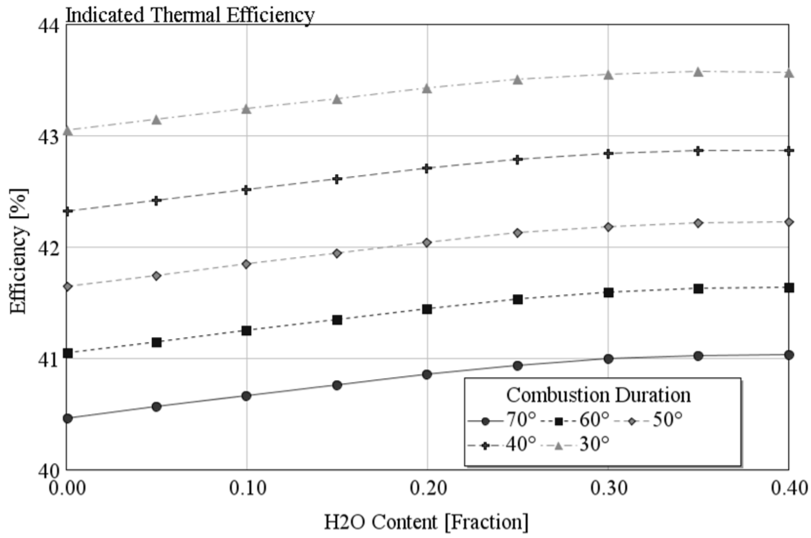


Figure 7 – Engine thermal efficiency

As maximum unburned zone temperature can be used as a knock onset indicator and assuming the initial 100% ethanol condition to be knock free, knock occurrence is not expected while water-in-ethanol content increases as the maximum unburned zone temperature decreases, as shown in figure 8 Other important fact is that the reduction in unburned zone temperature characterizes water as powerful anti-knock additive, something that would allow engine improvements in the search for increased efficiency.

Since in real engines operation it is expected that combustion becomes slower, with increased water-in-ethanol content, a plausible exercise would be as follows: an engine running on100% ethanol with combustion duration of 30º. The same engine when using, for example, 20% water-in-ethanol would possibly have a combustion duration of 60°. This would lead to a decrease from 43,04% to 41,44% in indicated thermal efficiency, leading to a higher fuel consumption, a fact that could be offset by the reduced production cost of such an ethanol concentration of 80% due to a net energy gain in production from about 45,15% (figure 1) – a net energy gain from 9,7% to 54,85%.

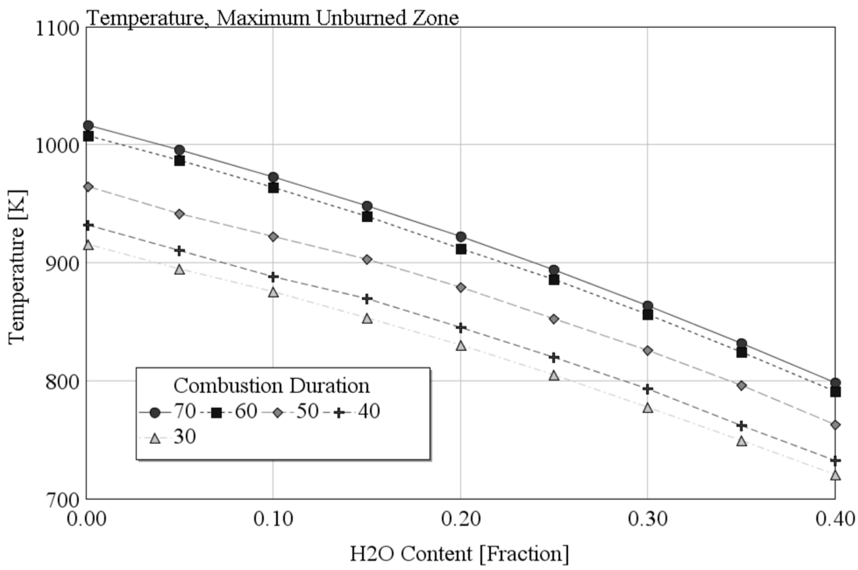


Figure 8 – Maximum Unburned Zone Temperature

## 4. CONCLUSION

This paper investigated performance and combustion behaviour of a SI engine running on different water-in-ethanol contents. Water enhances engine thermal efficiency as a combination of heat transfer reduction from gases to cylinder and volumetric efficiency enhancement while water-in-ethanol content increases. It is shown that water works well as a antiknock additive since it reduces the unburned zone temperature.

Morevoer, the growth in the energy lost in the exhaust process combined to the reduction of unburned zone temperature with the increase of water-in-ethanol concentration enables the use of high-pressure turbocharging, which would recover exhaust energy in high efficiency applications with a high degree of knock tolerance Also, this increased exhaust energy could be potentially used in combined heat and power applications (CHP) with the use of proper heat recovery systems.

## 5. ACKNOWLEDGEMENTS

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