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CFD and Emissions Modelling

Alternative Fuels Combustion Modelling (ACHA7002)

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Date (04/2026)

1. Introduction

Objectives

The main objective of this project is to present an alternative fuel option for the ignition combustion engines due to the new emissions regulation that would be implement on the European Union from 2035.

Emission regulation

Regarding the regulations, the laws that are going to be taken into account are the Euro 7, despite it will be implemented from January 2027 as the project focus on a possible scenario in the future, and Regulation (EU) 2019/631 focus on the CO₂ emissions. In the following graphs (Figures 1.1 & 1.2), it can be seen the tendency from previous years on how the limit for engine emissions has been going down.

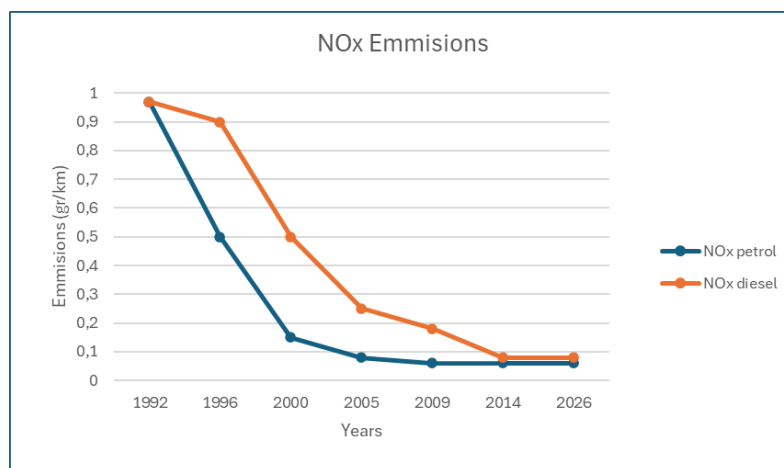


Figure 1.1. NOx emission regulations

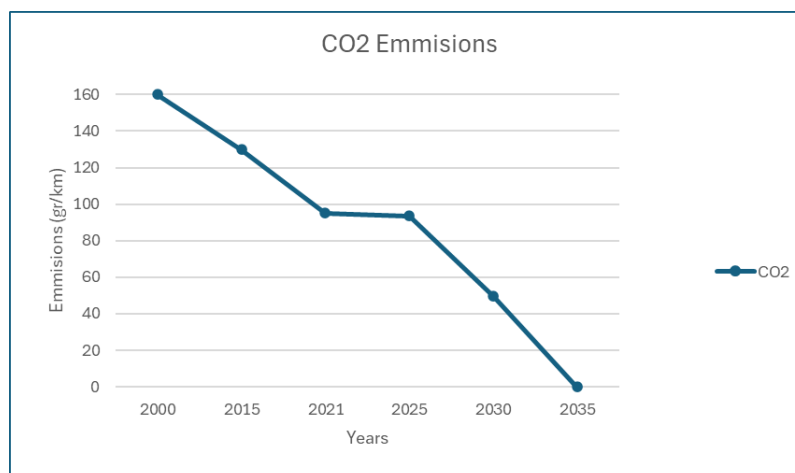


Figure 1.2. CO2 emission regulations

Analysing the data, the CO₂ emissions in the last years have been decreasing with bigger steps compared to NO_x emissions. As the regulation establishes, by 2035 CO₂ emission must be zero in new models. However, regarding NO_x emission, Euro 7 presents a limit that, at this moment, does not seem to be changed in the near future, as for the past years the limit has been maintained.

This context opens the opportunity to implement and search for non-carbon base fuels that can work in the future regulations.

Fuel selection

With the opportunity for non-carbon base fuels, a small literature review was completed with the objective of searching for power sources that are starting to get attention.

Here it comes the Ammonia, this non-carbon base chemical substance has been gaining a lot of attention in the latest years. The reasons behind come from different studies investigating its application in IC engines. These researches present Ammonia's performance and emissions (Lhuillier et al. 2019), its viability in the automotive sector comparing its efficiency and autonomy range against other fuels (Novella et al. 2023) and background around properties and production (Jadhav et al. 2026).

One of the most interesting aspects from the articles is that, in case the ammonia is produced with renewable energies, it could be the lowest producer of GHG-100 emissions in Cradle-to-grave cycle through an expected vehicle lifetime of 150,000 km (Novella et al. 2023).

However, the ammonia presents different challenges for its adaptation on the IC engines. Firstly, it is its combustion properties, as the chemical substance has a slow flame velocity and a high ignition temperature. These difficulties could be solved with the addition of a Hydrogen concentration, that would help accelerate the flame and lower the energy required to ignite (Lhuillier et al. 2019).

The other challenge of ammonia as a fuel are the Nox emission produce during its combustion. This is the major challenge for its implementation on ICE, as presented before, current and future regulations have a lower Nox emission limit. Different analysis has been developed to search for methodologies to reduces ammonia combustion's emission, for instance, a stoichiometry mixture with high pressure values reduces significantly the Nox emission (Lhuillier et al. 2019), on the other hand, adding Hydrogen contribute for its production (Lhuillier et al. 2019). Therefore, there must be a trade-off between all these variables to meet up with the regulations.

2. ANSYS Forte

Methodology

With the objective of perform a combustion simulation of a SI engine with ammonia as a fuel to be able to understand its characteristics, the analyses will be run with ANSYS Forte.

The engine model that will be use as a baseline configuration is a Jaguar V8 petrol supercharged. There are arguments to uses this model as the engine to perform the simulations with the ammonia. Firstly, SI engines seem to have a better performance with ammonia than CI engines (Lhuillier et al. 2019), as the spark ignition helps to achieve the combustion of the ammonia who has a high ignition temperature.

In relation with the supercharged technology, different studies present benefits from higher values of pressure on the combustion of ammonia (Lhuillier et al. 2019), such as a reduction on NOx emissions, higher efficiency and power. One of the references consulted (Lhuillier et al. 2019) suggest the study of supercharged technology as a new gap to expand the performance of ammonia as a fuel on ICE engines because, with higher pressure values, there is a tendency of greater results.

Talking about the set-up configuration for the simulations, with the aim of being efficient with the computer resources and time, the geometry and mesh implement will be defined on a quarter portion of one cylinder of the engine.

Following with the set-up models implement in the simulation, there are the spray model and spark model. The configuration of these models can be seen from Figures 2.1 to 2.4, where the main characteristics are based on previous studies (Jadhav et al. 2026; Lhuillier et al. 2019; Novella et al. 2023), for example the injection temperature needs to be high to prevent cooling the mixture and failing the ignition.

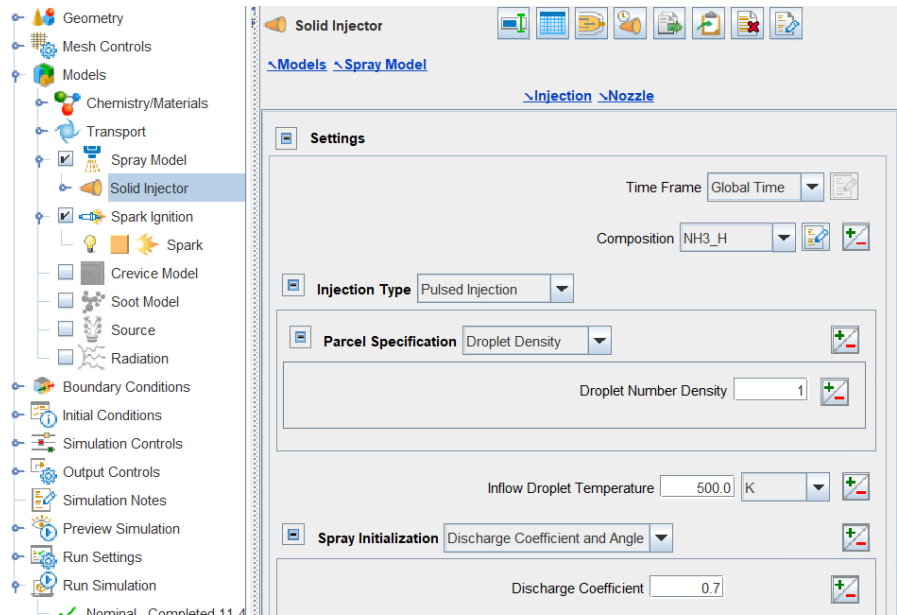


Figure 2.1. Injector configuration part 1.

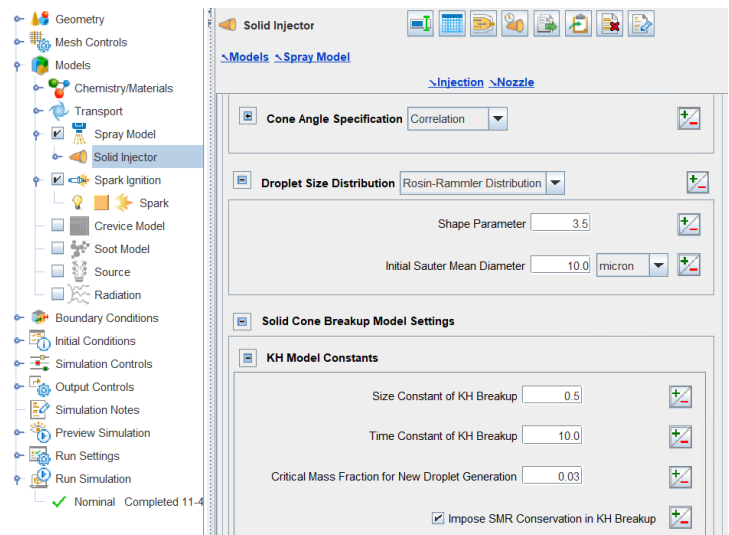


Figure 2.2. Injector configuration part 2.

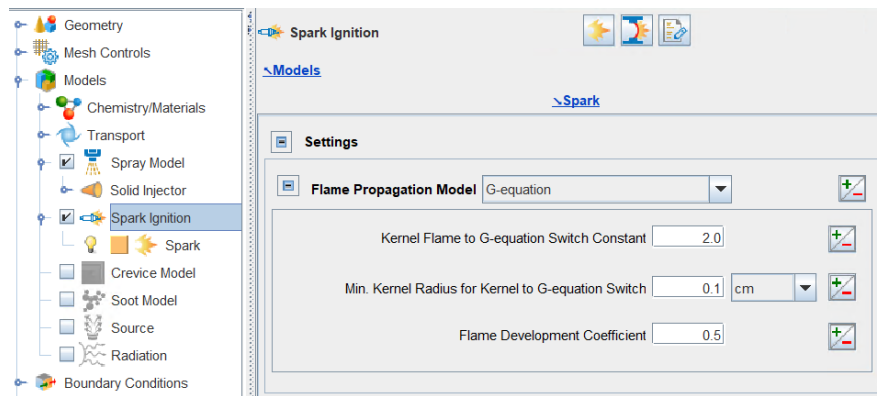


Figure 2.3. Spark configuration part 1.

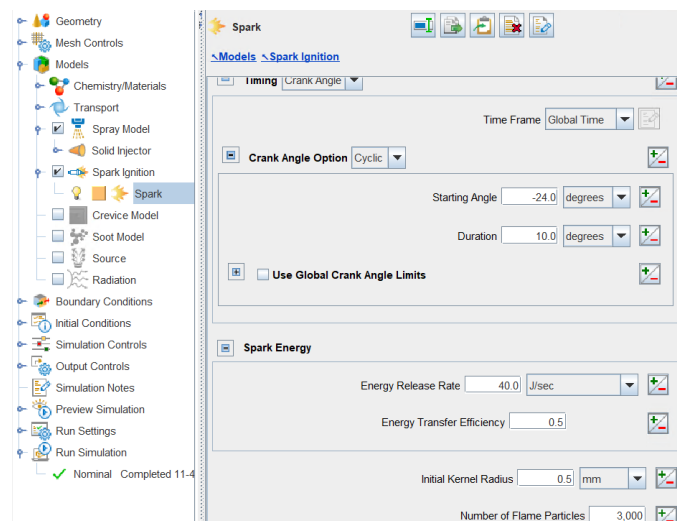


Figure 2.4. Spark configuration part 2.

The boundary conditions define for the set-up simulations are presented from Figures 2.5 to 2.9. These conditions are established from the baseline model of the Jaguar V8 petrol supercharged, as this is the engine use for the project.

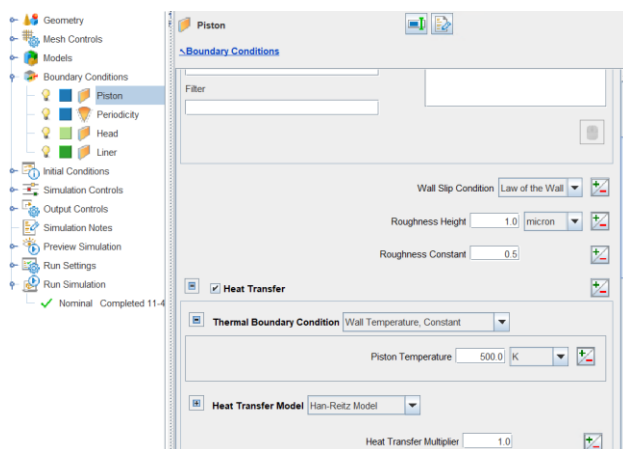


Figure 2.5. Piston configuration part 1.

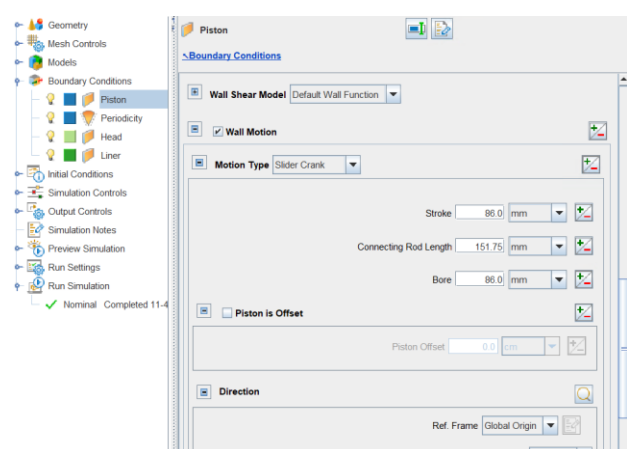


Figure 2.6. Piston configuration part 2.

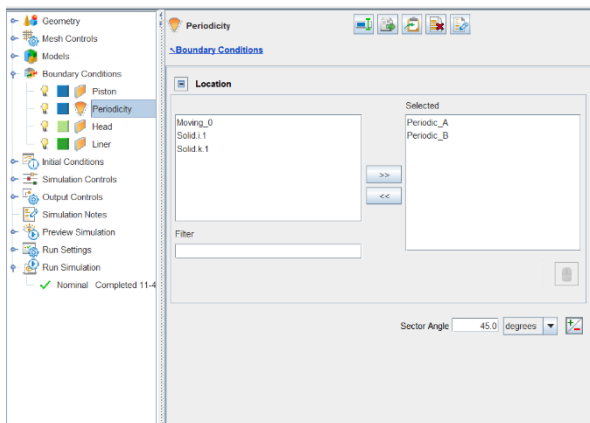


Figure 2.7. Periodicity configuration.

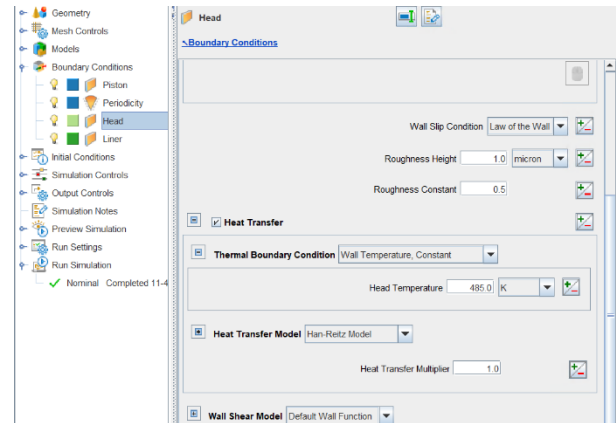


Figure 2.8. Head configuration.

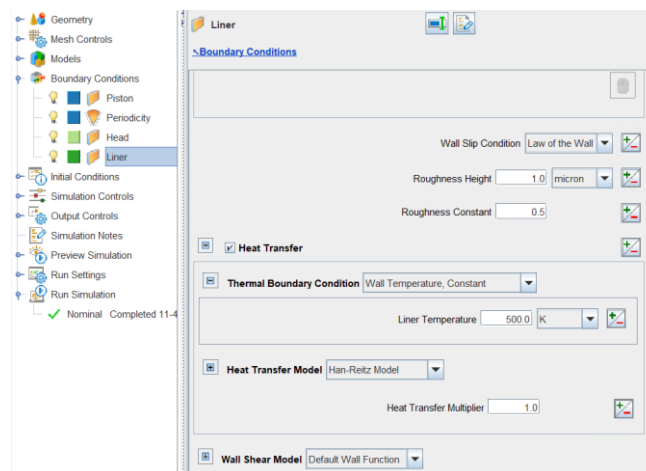


Figure 2.9. Liner configuration.

Finally, for the initial conditions of the simulation, they are presented on the Figure 2.10. For the initial mixture, it is built as a combination of air, hydrogen and small amount of ammonia on it. With the objective of evaluate the context of a combustion with a previous cycle completed.

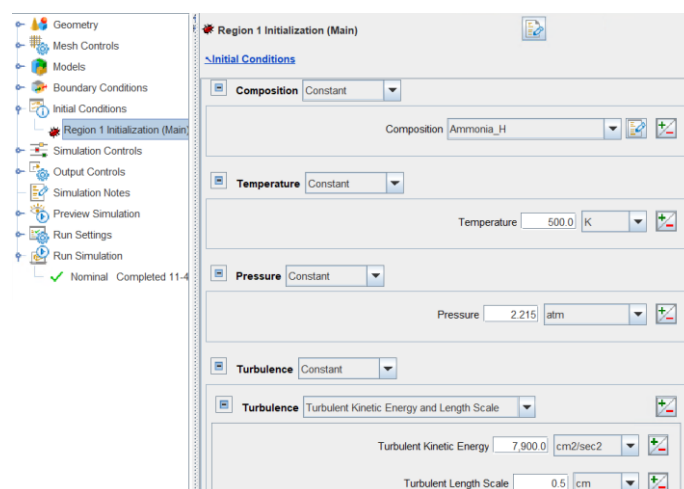


Figure 2.10. Initial conditions configuration.

There are different values of interest that are important to analyse to understand how they affect the combustion and obtain competitive results that support the use of ammonia as a fuel. These variables will be the concentration of hydrogen, the amount of ammonia injected and the pressure of the cylinder.

Results

After performing the simulations, the results of each value of interest are presented and the conclusions obtained from them.

The first parameter that was studied is the hydrogen concentration, as it was mentioned before, hydrogen helps to increase the flame speed and the ignition of the combustion, but also to decrease the emissions of NO_x as the table 1.1 presents. The results are aligned with the information in Lhuillier et al. 2019, where this tendency goes from bigger steps to smaller changes as the hydrogen concentration gets around 10-15%. The analysis of this variable was performed in all cases with the context of 3 mg of NH₃ injected, 2.215 atm of pressure and 500K

Table 1.1. Emissions vs H2 concentration

%H2	NOx (gr/ kg-fuel)	NH3 slip (gr/kg-fuel)
3%	126,8	0
5%	34,19	0,00024
10%	12,6	0,0019

The second parameter studied was the amount of ammonia injected. As the table 1.2 presents, reasonable results come up with the increase of the amount of fuel introduce, higher values of NO_x emissions. The tendency helps to confirm the set up and model developed are working correctly. The analysis of this variable was developed with an 10% of H₂ concentration, 2.215 atm of pressure and 500K.

Table 1.2. Emissions vs fuel injection.

Fuel inject (mg)	NOx (g/ kg-fuel)	NH3 slip (g/kg-fuel)
3	12,6	0,0019
5	14,13	0,0014
8	16,4	0,0015

The third parameter analysed was the pressure on the cylinder. This study came up because of in the literature (Lhuillier et al. 2019) it is suggested the implementation of supercharged technology and the investigation with higher pressure. The results are presented in the table 1.3. Analysing them, it seems in higher values of pressure there is not a big reduction of the emissions, although from values around 0.6 to 1.2 atm there was an important reduction (Lhuillier et al. 2019). It is in the range of 3-4 atm where there is an important reduction of NO_x emissions, but also and increase on the fuel unburned. However, 3-4 atm of pressure are values out of range for our model, but not for ammonia because of its higher ignition temperature it could achieve greater values of pressure before combusting. This opportunity requires further investigation and complex simulations out of this project, nevertheless it is a potential area of development.

Table 1.3. Emission vs Initial Pressure

Pressure (atm)	NO _x (gr/ kg-fuel)	NH ₃ slip (gr/kg-fuel)
1,8	12,55	0,0011
2,215	14,13	0,0014
2,5	13,1	0,002
3	11,14	0,0034
4	6,23	0,0053

After all this process, it seems the configuration that has the better balance will be with the conditions of 10% of H₂, 5 mg of ammonia injected, temperature of 500K and 2.5 atm of pressure.

Following this set up, its pressure and HRR graph are presented in figures 2.11 & 2.13. Regarding the pressure data, the shape of the graph helps to validate the model and simulations as it gets near to the distribution of an SI engine. However, there are differences on the smoothed and accuracy of the model and data because of the limitations on the computer resources.

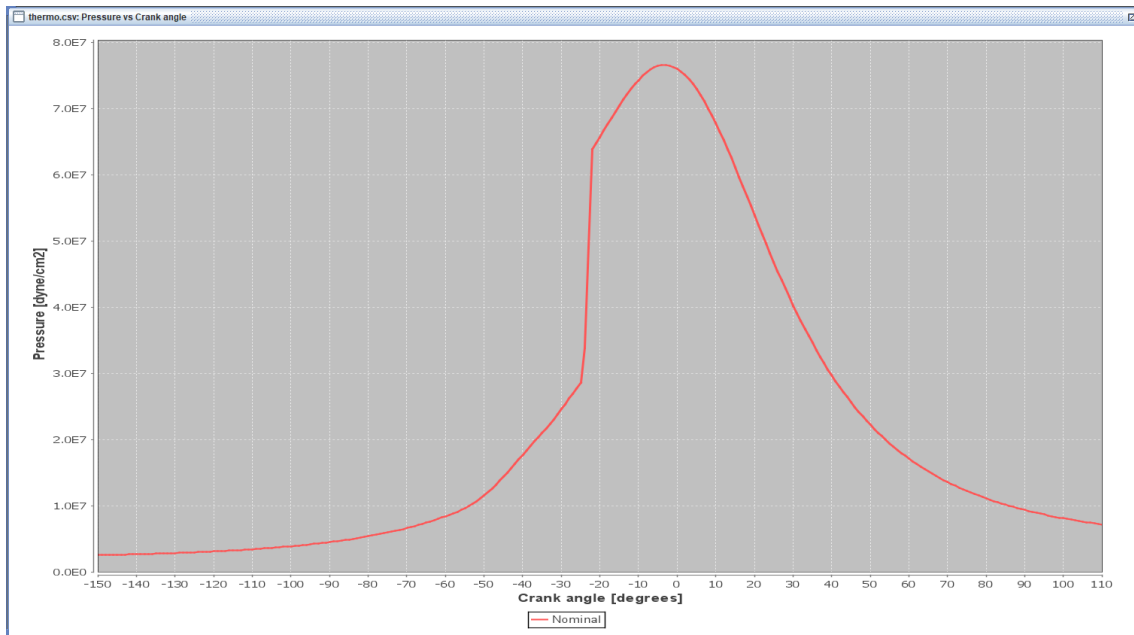


Figure 2.11. Pressure evolution vs CA in ammonia engine.

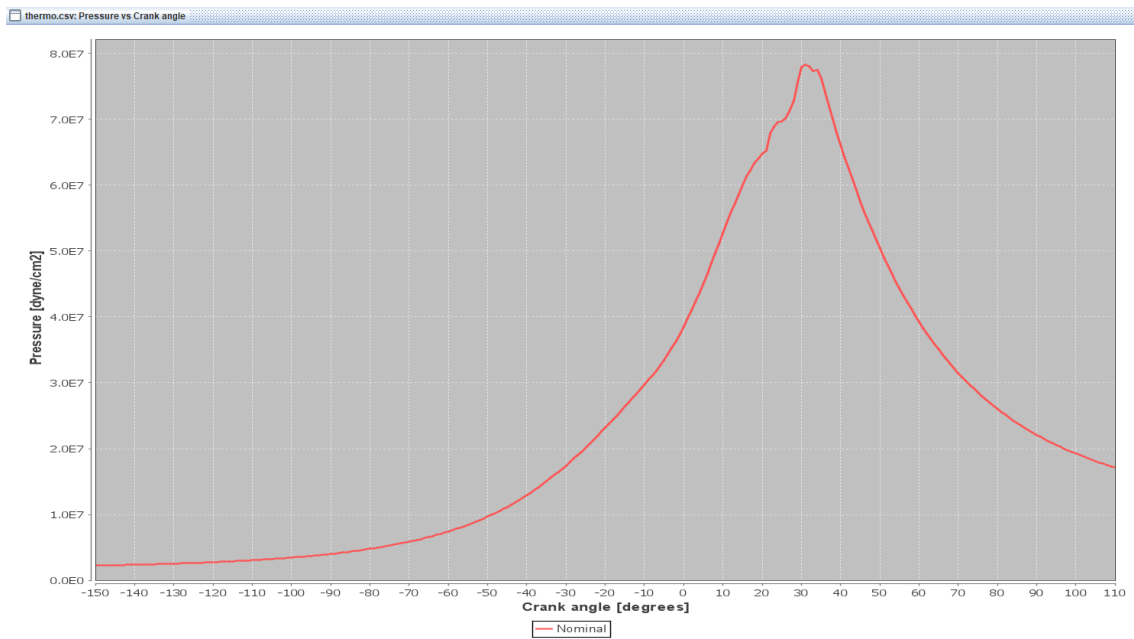


Figure 2.12. Pressure evolution vs CA in petrol engine.

These limitations stand out more in the HRR (Heat release rate), as the graph has an aggressive and quicker shape that differs with the theoretical one (Novella et al. 2023). Although, this quicker and aggressive performance could be justified with the hydrogen concentration that accelerates the flame speed and increase the energy, it seems to be more focus on the quality of the mesh to be able to calculate the values in a complex combustion.

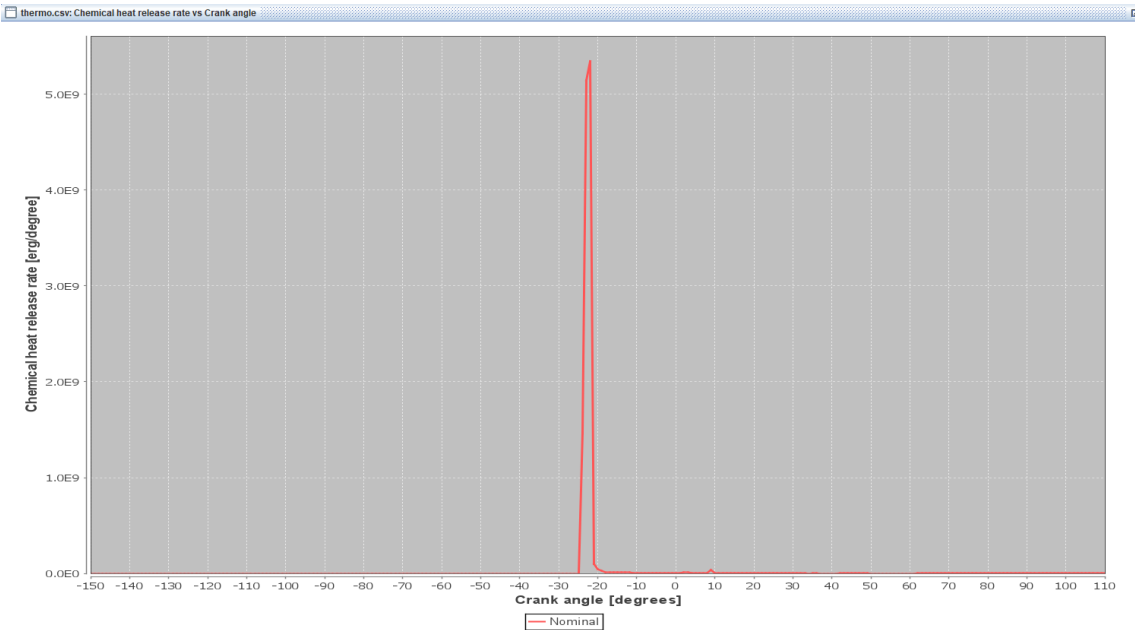


Figure 2.13. HRR vs CA in ammonia engine.

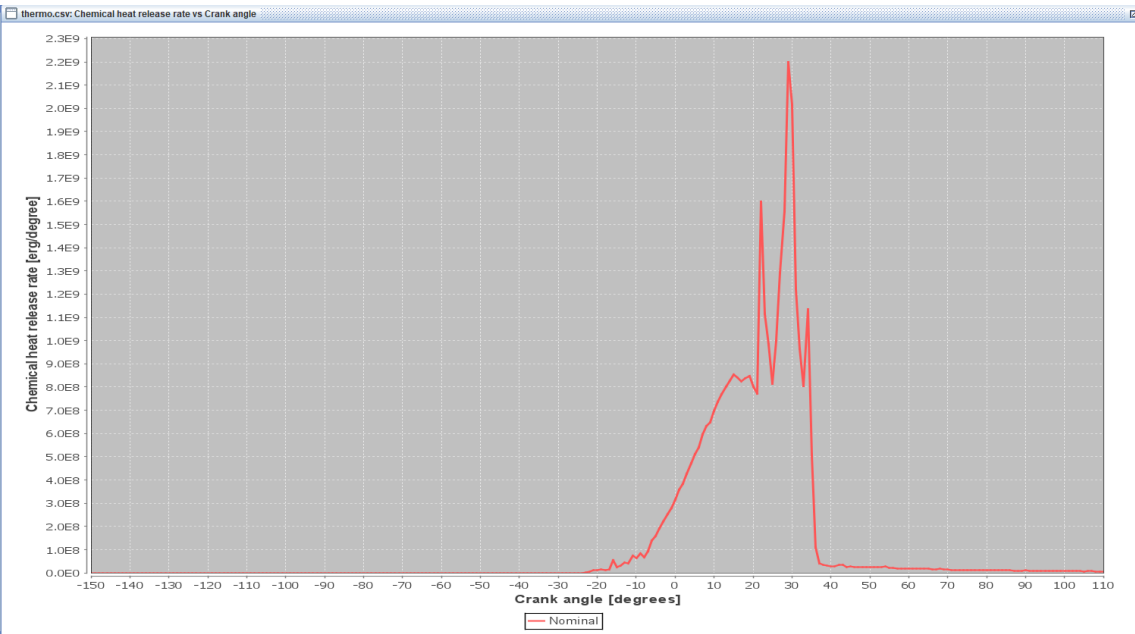


Figure 2.14. HRR vs CA in petrol engine.

3. Ricardo WAVE

Methodology

Ricardo WAVE software will be used to implement the data and combustion model from ANSYS Forte simulations into a real engine environment. In this case, for this project the main focus is the emissions, restricted by the regulations mentioned before. Therefore, the set up develop will be model as a 1D cylinder to reduce the computer resources demand as the objective of this project is to present a possible alternative of ICE for the future regulations.

In the following figures 3.1 to 3.5, it is presented the configuration of the main parameters of the set up and the model design.

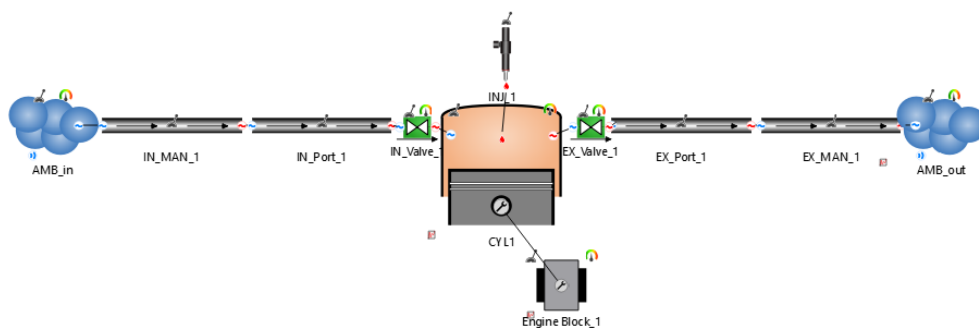


Figure 3.1. WAVE single cylinder design.

Label: Engine Block_1

Engine Block Data | Advanced | RT Modelling | Cooled Elements | Sensors / Ac

General

Engine shape: Inline

Mixture type: Homogeneous (SI)

Strokes per cycle: 4

Number of cylinders: 1

Firing Order and Relative TDC

Order	Cylinder	TDC [deg]
1.	CYL1	0

Operating Condition

Engine speed: Speed

Reference temperature: 500 K

Reference pressure: 2.5 atm

Reference Location for Plenum Volumetric Efficiency

Figure 3.2. Engine block configuration.

Geometry

Bore: 86 mm

Crank Stroke: 86 mm

Clearance height: 2 mm

Head area multiplier: 1

Piston area multiplier: 1

☐ Sinusoidal Movement

Connecting rod length: 151.75 mm

Pin offset: 0 mm

Compression ratio: 10

☐ Swirl Prediction

Boundary Conditions

Piston: 500 K

Liner: 500 K

Head: 485 K

Intake valve: 400 K

Exhaust valve: 450 K

Figure 3.3. Cylinder configuration.

Figure 3.4. Injector configuration.

Figure 3.5. Model properties configuration.

As it can be seen the majority of the parameters are define from Forte and implemented. The only one define in WAVE is the fuel/air ratio with a value of 0.12 to make a lean mixture, the reason behind this selection is that, based on a previous study (Lhuillier et al. 2019), lean proportions help to increase the efficiency of the engine.

In relation with the configuration of other parts of the model, such us the valves, ducts, ambient and exhaust air; they are established with standard parameters define form WAVE for SI engines as their influence does not make an important difference on the results considering the low grade of complex from this simulation.

Results

After completing the simulation, that was perform from 1000 rpm to 6000 rpm by steps of 1000, there are conclusions obtained from it that will be presented in the following figures below. Firstly, it is show the pressure evolution (figure 3.6) in the cylinder for one cycle at 2000 rpm, as it can be seen the shape of the graph is align with the ones obtained in Forte for the ammonia and petrol engines, that helps to validate the model from Forte and the set up as the pressure have a similar behaviour near the reality.

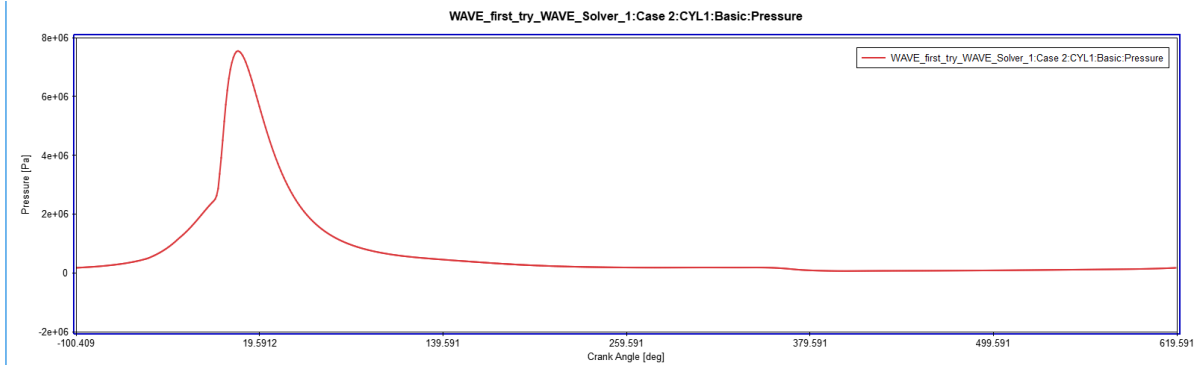


Figure 3.6. Pressure vs CA in ammonia engine at 2000 rpm.

Secondly, in figure 3.7, it can be shown the NO_x emissions from the engine at the different velocities simulated. The ones to take more into consideration will be the values at 2000 and 3000 rpm, as this is the range where the engines should perform. Analysing the results, the range of values go around from 600 ppm to 750 ppm, these values must be converted to the same scale as the regulation Euro 7 limit to be able to compare them. Euro 7 limit is 0.06 gr/km, an approximation to ppm will be around 800-1000 ppm. Although the results seem to be below the limit, it is important to remark there are other important aspect to take into account that could affect the NO_x emissions, for example the other cylinders or the efficiency. However, there are post treatment methods (SCR) to reduce the emissions that could be implement and they are not consider in this project.

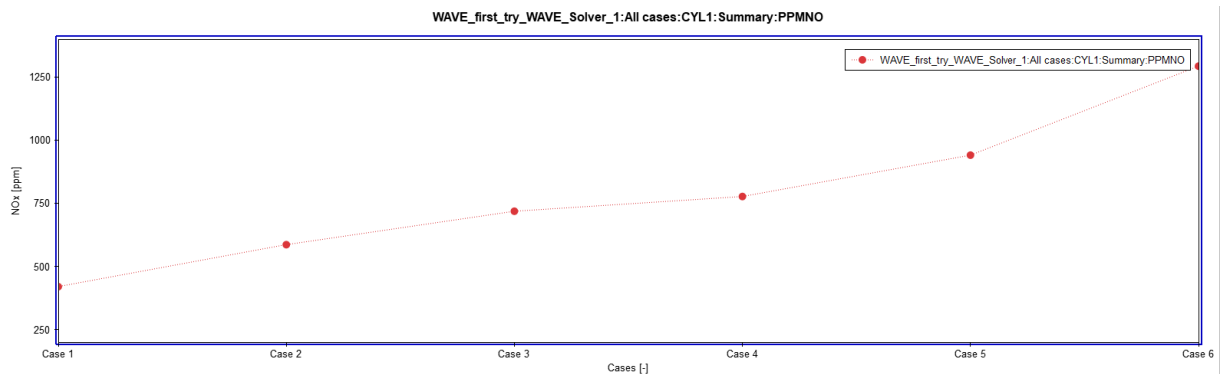


Figure 3.7. NO_x vs rpm in ammonia engine.

Finally, there are the brake power and the engine torque of the model developed in figures 3.8 & 3.9. As it can be seen, the engine torque has a logic behaviour with maximum values around 3000-4000 rpm and after that it starts to decrease. Talking about the brake power, the performance is not as expected, it is decreasing with higher rpm what indeed should keep increasing. The reason behind could be a slow combustion at high rpm where it does not take advantage of the whole expansion. This can be due to ammonia's low flame velocity or the imbalance of the model in some aspects. The methods that could be implemented to help to correct this behaviour are start the combustion early, increase the H₂ concentration or increase the fuel/air ratio, however most of them could lead in an emissions increase.

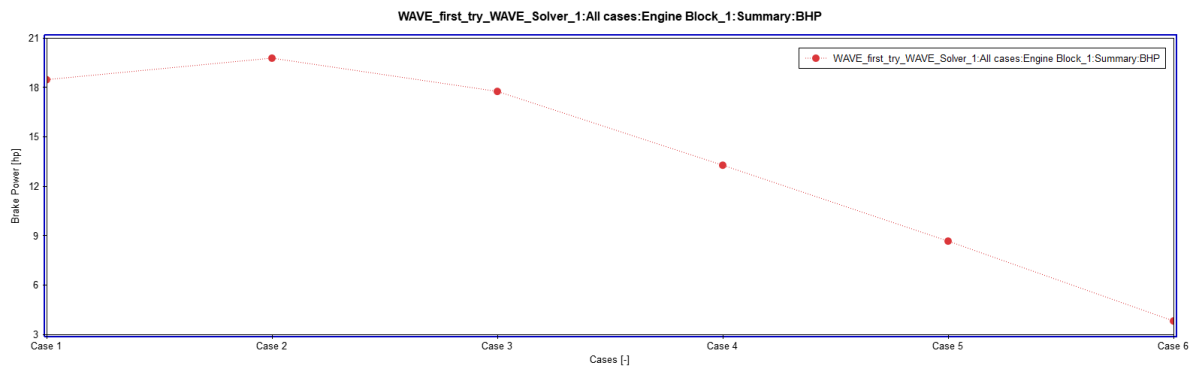


Figure 3.8. Brake power vs rpm in ammonia engine.

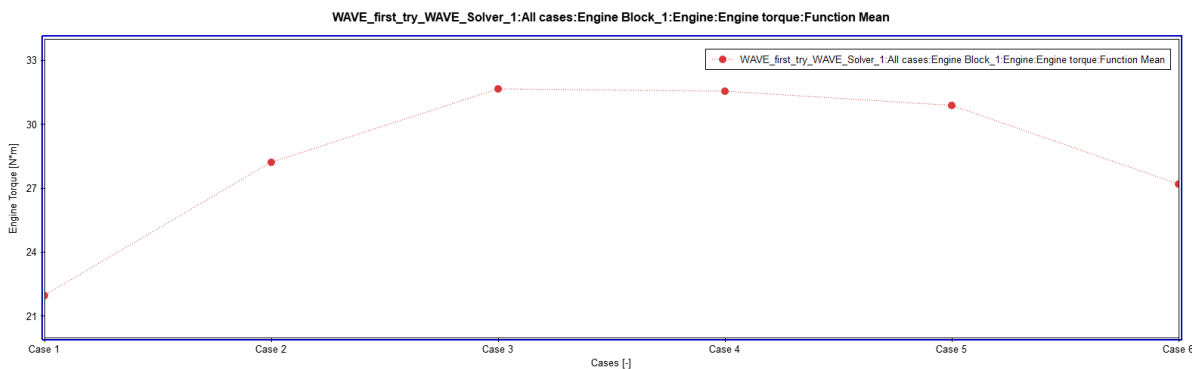


Figure 3.9. Engine torque vs rpm in ammonia engine.

Conclusions

There are different conclusions obtained from the project. Firstly, it is the potential that ammonia has as a fuel for IC engines combining with hydrogen to surpass some of its limitations. However, there are important challenges that require further studies and research to clarify the most efficient configuration for ammonia's implementation to achieve a competitive autonomy. One of the biggest advantages for ammonia is to be a non-carbon base product, therefore, it can work with the strictest regulations in 2035.

Another conclusion obtained is the limitations on this project regarding the simulations. This point affects directly the performance of them and different assumptions has been considered to develop a first analysis of the characteristics of the model. The mesh design and boundary conditions establish affects directly the results and for further investigation more complex set ups should be developed to achieve a realistic accuracy.

References

- Jadhav, A., Bandyopadhyay, D., Sutar, P.S., Sonawane, S.B. et al., "The Viability of Ammonia in the Automotive Sector: Challenges and Opportunities," SAE Technical Paper 2026-26-0128, 2026, doi:10.4271/2026-26-0128. (Jadhav et al. 2026)
- Lhuillier, C., BREQUIGNY, P., Contino, F., and Rousselle, C., "Performance and Emissions of an Ammonia-Fueled SI Engine with Hydrogen Enrichment," SAE Technical Paper 2019-24-0137, 2019, doi:10.4271/2019-24-0137. (Lhuillier et al. 2019)
- Novella, R., Pastor, J., Gomez-Soriano, J., and Bayona, J.S., "Challenges and Directions of Using Ammonia as an Alternative Fuel for Internal Combustion Engines," SAE Technical Paper 2023-01-0324, 2023, doi:10.4271/2023-01-0324. (Novella et al. 2023)
- Climate Action. (2019). *Cars and vans*. [online] Available at: https://climate.ec.europa.eu/eu-action/transport-decarbonisation/road-transport/cars-and-vans_en.