Designing an Ammonia-compatible Fuel Injector for retrofitting current Internal Combustion Engines using CFD

PI: Tommaso Bocchietti, Department of Mechanical & Mechatronics Engineering, University of Waterloo
Contact: Tommaso Bocchietti, tbocchie@uwaterloo.ca
Date: March 20, 2024

Abstract The continuous emission of greenhouse gases from internal combustion engines is a major concern for the environment. The transportation sector is the second-largest source of greenhouse gas emissions in the world, preceded only by the energy sector.

In the past few years, some alternative to fossil fuel have been proposed, such as the adoption of electric vehicles, the use of methane, or the use of hydrogen. However, all of these alternatives have some drawbacks, such as the needs of a huge infrastructure to support the use of electric vehicles, or the high emissions of CO_2 from methane combustion, or the low energy density of gaseous hydrogen.

Ammonia instead is a promising alternative fuel, with a considerable energy density and no CO_2 emissions. However, the use of ammonia requires the development of new mechanical components that can handle its specific properties.

This research project aims to develop a new fuel injector suitable for ammonia, so that it can be retrofitted in existing Internal Combustion Engines (ICEs). The project will use Computational Fluid Dynamics (CFD) simulations to model the spray of Ammonia inside the combustion chamber, giving insights on the design of the new fuel injector.

Keywords Ammonia, Fuel Injector Design, Internal Combustion Engines, Computational Fluid Dynamics

1 Objectives and Impact

The growing concern about the environmental impact of the transportation sector has led to the search for alternative fuels.

Ammonia has the potential to be the fuel of the future, as it has a considerable energy density (Table 1) and does not produce CO_2 emissions when burned. However, Ammonia might also have a negative impact on the environment, as it can be the source of NO_x emissions[1]. The latter can be mitigated by using a proper combustion strategy, controlling in particular the temperature of the combustion chamber and the ratio air-to-fuel[1].

In this research project, we propose a methodology that at the end would lead to a new design for a fuel injector that can allow the use of Ammonia in the current internal combustion engines (ICEs). Our goal is to develop a fuel injector that can be retrofitted in existing ICEs, so that the transition to Ammonia can be smooth and cost-effective. Ideally, but depending on the intermediate results of the project, the new fuel injector will be designed keeping all the parameters of the current (gasoline or diesel, depending on the best compatibility we will discover) ICE untouched, so that no other modification to the engine will be required expect for the fuel injector itself.

The impact of this research project is potentially huge. At the time this proposal is written, some research projects([5, 7]) are ongoing towards the "green Ammonia" production, underlining the importance of this molecule and potentially making it the key to a sustainable future. In case of success, the transportation sector will be able to use a fuel that has a medium energy density compared to the traditional gasoline and diesel, but that does not produce CO_2 emissions.

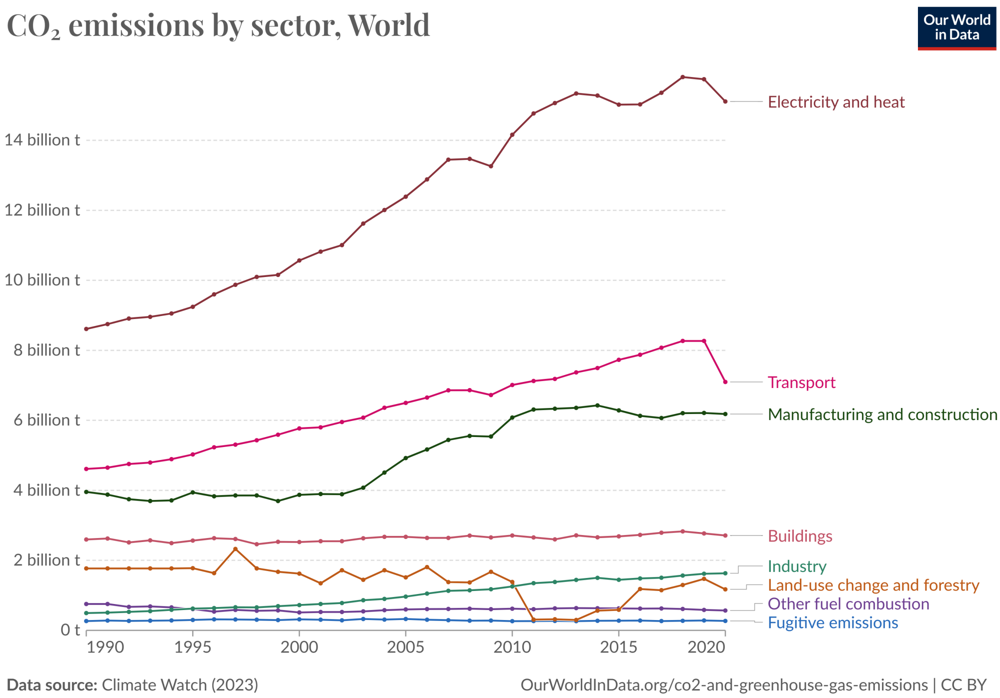

Figure 1: CO_2 emission by sector[9]. Transportation is the second-largest source.

	Liquid Ammonia	**Gasoline**	**Diesel**
Volumetric [GJm^{-3}]	11.38	30.6	37.2
Gravimetric [$MJKg^{-1}$]	18.65	43.6	44.8

Table 1: Energy density of Ammonia compared to traditional fuels[2].

2 Background

So far, just some "entry-level" investigation on the feasibility of using Ammonia as a fuel has been done. In particular, we would like to mention the work of:

- **R. Pelé et al.[8]**: a visual inspection of the spray geometry of Ammonia has been conducted, showing multiple similarity with the spray of gasoline and diesel under various conditions of temperature and pressure of air. Some empirical correlations have been proposed to predict the penetration and angle of the spray, but no CFD simulations have been conducted.
- **K.D.K.A. Somarathne et al.[10]**: a first CFD modelling of a simple non-reactive condition of the spray of Ammonia has been conducted. A particular attention to the flash-boiling[1] condition was given, and the results showed a good agreement with the experimental data.
- **J. Wang, F. Dalla Barba[11]**: a more advanced CFD simulation of the spray of Ammonia (still in a non-reactive condition) has been conducted. The authors proposed the parcel model[2] strategy to reduce the computational cost of the simulation, while still obtaining a good agreement with the expected results. Coarsening mesh and the use of the Eulerian-Lagrangian approach were also proposed to further reduce the computational cost.

Moreover, studies from E.C. Okafor et al.[6] have also demonstrated the feasibility of using Ammonia in a turbine engine, showing that the combustion of Ammonia can be stable and efficient; while A.

[1]Flash-boiling is the process of a liquid turning into a gas when its pressure is suddenly reduced[4].

[2]The parcel model is a strategy to reduce the computational cost of the simulation, by grouping particles with similar properties such as diameter, velocity, position, shape and solving the equations for the group instead of for each particle.

Hayakawa et al.[3] demonstrated the feasibility of a co-firing strategy of Ammonia with Hydrogen and air.

The main challenges in the use of Ammonia as a fuel are the high ignition temperature (around $650°C$), the slow flame speed, and the possible formation of $\mathrm{NO_x}$ emissions.

However, we believe that the importance of the use of Ammonia as a fuel is so high that it is worth to invest time and resources in the development of a new fuel injector that can handle the specific properties of Ammonia and that can be retrofitted in existing ICEs.

3 Research Plan and Methodology

Our research project aims to develop a new fuel injector suitable for Ammonia, so that it can be retrofitted in existing ICEs.

We will make use Computational Fluid Dynamics (CFD) simulations as a tool to simulate the conditions of the spray of Ammonia in the combustion chamber, allowing us to test different designs of the fuel injector without the need of building a physical prototype, which would be time-consuming and expensive.

We are conscious that the development of a new fuel injector is a complex task, and the modelling of Ammonia kinematics and combustion is not trivial. For this reason, we have divided the research project into three major phases, each one with its own specific objectives and expected results.

3.1 Phase 1: CFD Modelling of the Spray of Ammonia in a Non-Reactive Condition

The first phase of the research project aims to recreate and possibly improve the CFD model that can be found in the literature, which simulates the spray of Ammonia in a non-reactive condition. In particular, at the end of the phase we expect to have a CFD model that can accurately predict the characteristics of the spray of Ammonia such as droplet size, velocity, distribution, penetration..., given the environmental conditions and domain restrictions.

In particular, we can further divide the objectives of this phase into the following tasks:

1. **Literature Review:** a deep review of the state of the art about the modelling of the spray of Ammonia is required before starting the development of our CFD model. This will allow us to understand the limitations of the existing models and to identify the key parameters that need to be considered.
2. **Development & Validation of the CFD Model:** the development of the CFD model will be carried out using commercial software as `OpenFOAM` and `ANSYS Chemkin`. The model will be validated against the experimental data available in the literature. Based on the information already available, we can already hypothesize that the model will be based on the Eulerian-Lagrangian approach, where the Eulerian solver is dedicated to advance in time the flow field, while the Lagrangian solver is used to evaluate the mass, momentum and energy equations of the single parcel[2].

Once our model is validated against the experimental data available in the literature, we can proceed to the next phase of the research project.

3.2 Phase 2: CFD Modelling of the Spray of Ammonia in a Reactive Condition

The second phase of the research project aims to extend the CFD model developed in the previous phase to a reactive condition.

Given that, to our current knowledge, no experimental data exists about the reactive condition of Ammonia spray in literature, we will need to perform an experimental campaign to gather the necessary data to validate our model. To do so, we will try to replicate the conditions of the combustion chamber of an ICE, and measure the quantity of interest such as the temperature, pressure, and flow rate. This implies the use of a test bench equipped with (at least) a combustion chamber, a fuel injector, and a spark plug, as well as the necessary sensors and data acquisition systems.

In particular, we can further divide the objectives of this phase into the following tasks:

1. **Experimental setup:** the experimental setup will be designed to replicate the conditions of the combustion chamber of an ICE. At first, an open domain will be used with an external spark plug to ignite the Ammonia. At the second stage, the setup will be enclosed to further replicate the conditions of a real combustion chamber.
2. **Data acquisition & analysis:** the experimental campaign will be carried out to gather the necessary data to validate our CFD model. The data will be processed, analyzed and compared with the results of the CFD simulations. In the analysis phase, a use of Machine Learning algorithms can be considered to increase the possibility to find correlations across the data set and improve the accuracy of the model.

As in the first phase of the project, the model developing will be carried out using commercial software as `OpenFOAM` and `ANSYS Chemkin`.

Once our model for reactive condition is ready and validated, we can proceed to the next phase of the research project.

3.3 Phase 3: Design and Testing of the New Fuel Injector

The third phase of the research project aims to design the new fuel injector suitable for Ammonia, and to test it in a real ICE.

The design of the fuel injector will be based on the results of the CFD simulations, and it will be carried out using the CAD software `CATIA V5`.

Our driving motivation here is to design a fuel injector that can be retrofitted in existing ICEs, so that the transition from fossil fuels to Ammonia can be as smooth as possible.

In particular, we can further divide the objectives of this phase into the following tasks:

1. **Design of the Fuel Injector:** the design of the fuel injector will be based on the results of the CFD simulations. As domain, we will consider a Direct Injection system, where the fuel injector spray the Ammonia directly into the combustion chamber. Depending on the results from previous phases of the project, the design will start from the assumption that no other parameter of the ICE has to be modified (such as the pressure of the inlet and exhaust valves, the compression ratio, the ignition timing...). In case of evidence that some parameters have to be modified, we will also propose at the end of the project a set of guidelines to retrofit in existing ICEs.
2. **Testing of the Fuel Injector:** finally, a first prototype of the fuel injector will be built and tested in a real ICE. Using a similar setup as the one used in the experimental campaign of the second phase, we will measure the performance of the fuel injector in terms of spray characteristics, combustion efficiency, and emissions. The data will be processed, analyzed and compared with the prevision of the CFD simulations.

At the end of this phase, we expect to have a new fuel injector suitable for Ammonia, and a set of guidelines that can be used to retrofit existing ICEs.

4 Deliverables

The research is focused on the development of a new fuel injector suitable for Ammonia, so that it can be retrofitted in existing ICEs.

The main deliverables of the research project are:

- A CFD model that can accurately predict the characteristics of the spray of Ammonia in a non-reactive condition.
- A CFD model that can accurately predict the characteristics of the spray of Ammonia in a reactive condition.

- A first design/prototype of the new fuel injector suitable for Ammonia that can be retrofitted in existing ICEs.

If the research is successful, the impact would be huge as it would allow a fast transition from fossil fuels to Ammonia as a fuel for ICEs thus reducing the emissions of CO_2.

A References

[1] A. A, M. S, S. H, A. M, W. P, P. D, and V.-M. A. Evolution of ammonia reaction mechanisms and modeling parameters: A review. *Applications in Energy and Combustion Science*, 15:100175, 2023.

[2] L. Barelli, G. Bidini, and G. Cinti. Operation of a solid oxide fuel cell based power system with ammonia as a fuel: Experimental test and system design. *Energies*, 13:6173, 11 2020.

[3] A. Hayakawa, M. Hayashi, M. Kovaleva, G. J. Gotama, E. C. Okafor, S. Colson, S. Mashruk, A. Valera-Medina, T. Kudo, and H. Kobayashi. Experimental and numerical study of product gas and n2o emission characteristics of ammonia/hydrogen/air premixed laminar flames stabilized in a stagnation flow. *Proceedings of the Combustion Institute*, 39(2):1625–1633, 2023.

[4] M. Mojtabi, G. Wigley, and J. Helie. The effect of flash boiling on the atomization performance of gasoline direct injection multistream injectors. *Atomization and Sprays*, 24:467–493, 01 2014.

[5] O. A. Ojelade, S. F. Zaman, and B.-J. Ni. Green ammonia production technologies: A review of practical progress. *Journal of Environmental Management*, 342:118348, 2023.

[6] E. C. Okafor, H. Yamashita, A. Hayakawa, K. K. A. Somarathne, T. Kudo, T. Tsujimura, M. Uchida, S. Ito, and H. Kobayashi. Flame stability and emissions characteristics of liquid ammonia spray co-fired with methane in a single stage swirl combustor. *Fuel*, 287:119433, 2021.

[7] A. Olabi, M. A. Abdelkareem, M. Al-Murisi, N. Shehata, A. H. Alami, A. Radwan, T. Wilberforce, K.-J. Chae, and E. T. Sayed. Recent progress in green ammonia: Production, applications, assessment; barriers, and its role in achieving the sustainable development goals. *Energy Conversion and Management*, 277:116594, 2023.

[8] R. Pelé, C. Mounaïm-Rousselle, P. Bréquigny, C. Hespel, and J. Bellettre. First study on ammonia spray characteristics with a current gdi engine injector. *Fuels*, 2(3):253–271, 2021.

[9] H. Ritchie, P. Rosado, and M. Roser. Emissions by sector: where do greenhouse gases come from? *Our World in Data*, 2020.

[10] K. D. K. Somarathne, H. Yamashita, S. Colson, E. Okafor, A. Hayakawa, T. Kudo, and H. Kobayashi. Liquid ammonia spray combustion and emission characteristics with gaseous hydrogen/air co-firing. 12 2021.

[11] J. Wang and F. Dalla Barba. Assessment of the parcel model in evaporating turbulent diluted sprays within a large-eddy-simulation approach. *International Journal of Multiphase Flow*, 169:104609, 2023.