



Next-Generation Fuel in Internal Combustion Engine: Ammonia

Designing a Suitable Fuel Injector for Ammonia Using CFD

Tommaso Bocchietti

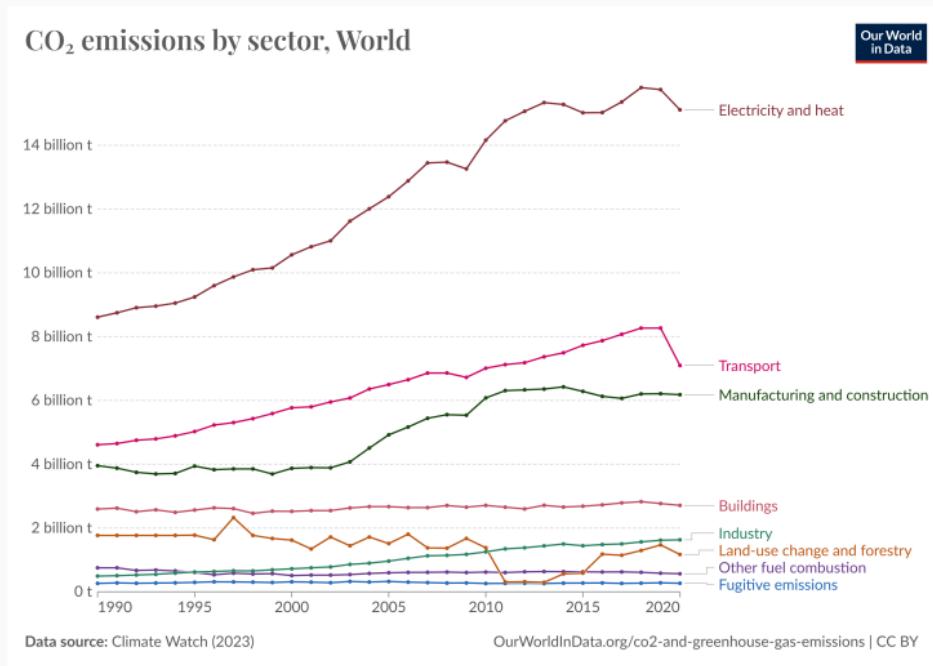
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University of Waterloo

Motivations

CO₂ Emission by Sector

Transportation sector is the second-largest contributor to CO₂ emission.



Transportation sector has been looking for alternative fuels to reduce CO₂ emission.

- **Electricity:** requires a large infrastructure to support the global demand
- **Methane:** worse than CO₂ in terms of greenhouse effect (short-term)
- **Hydrogen:** difficult to store and transport

Ammonia as a Fuel

Researchers started looking at Ammonia as a potential alternative fuel.

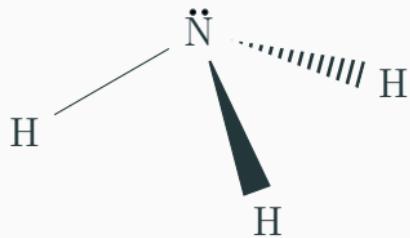


Figure 1: Ammonia molecule (NH_3)

Advantages of Ammonia:

- No carbon content (zero CO_2 emission)
- Long history of use in the chemical industry
- Possible use as hydrogen carrier

Ammonia as a Fuel



DIESEL



GASOLINE



METHANE



AMMONIA

Disadvantages of Ammonia (also based on NFPA¹):

- Least flammable source, which also suggest **slow flame speed**
- Its combustion might produce **high NO_x emissions** if not properly controlled

¹National Fire Protection Association 704: Standard System for the Identification of the Hazards of Materials for Emergency Response

Research Focus

Fuel injector for Ammonia

Design a **direct Ammonia fuel injector compatible with current internal combustion engines.**

The key factors driving our design will be:

- Stable flame inside the combustion chamber
- Low-to-zero NO_x emissions

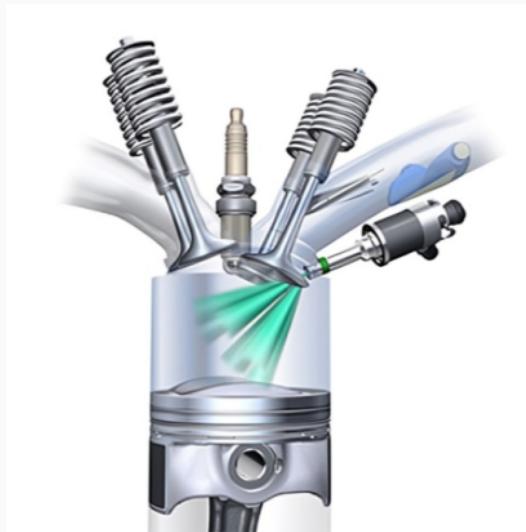


Figure 2: Direct fuel injection in internal combustion engines

Fuel injector for Ammonia

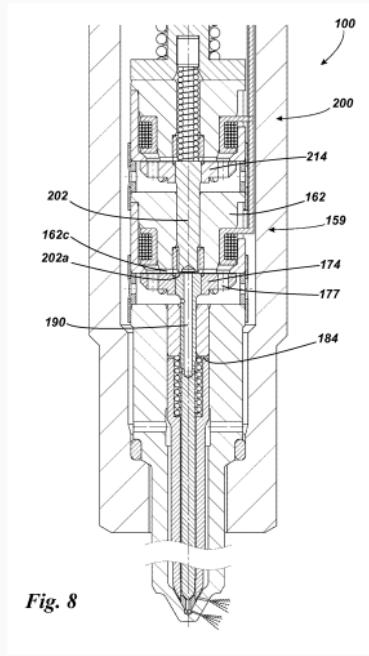


Figure 3: "Fuel injector"
(US20120080011A1)

The core focus will be on the **controllability of the atomization process**.

Given that, we also need to take into account the environmental working conditions:

- Temperatures (inlet, chamber, exhaust)
- Pressures (inlet, chamber, exhaust)
- Air-fuel ratio
- Injection timing

Prior Studies

Title: First Study on Ammonia Spray Characteristics with a Current GDI Engine Injector

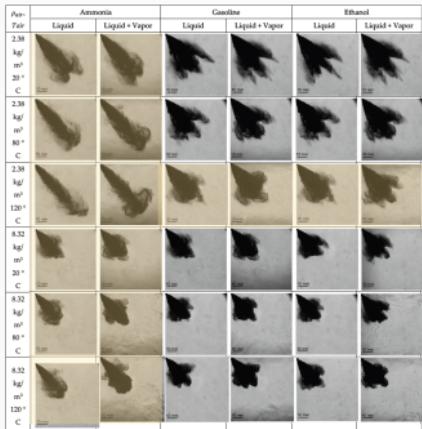


Figure 4: Comparison of spray shape (different fuels & conditions).

Geometrical spray characteristics analysis of Ammonia compared to Gasoline & Ethanol.
Conclusions:

- Ammonia spray is longer and thinner.
- Spray angle maximum at P_{sat} .
- Empirical correlation for $spray_L(t)$ proposed.

In general, the study enhanced the possibility for the use of Ammonia in GDI engines.

Title: Liquid Ammonia Spray Combustion and Emission Characteristics with Gaseous Hydrogen/air Co-firing

A **numerical model** for LNH₃¹ combustion was developed and validated (LES² based). Particular attention to the **flash-boiling condition** modelling was given.

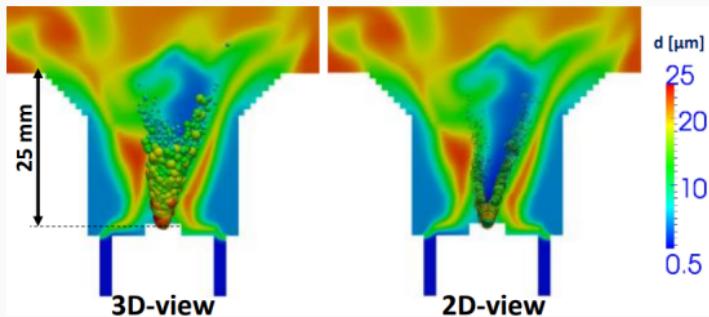


Figure 5: 3D and 2D views of LNH₃ droplet distributions.

¹LNH₃: Liquid Ammonia

²LES: Large Eddy Simulation

Title: Assessment of the parcel model in evaporating turbulent diluted sprays within a Large-Eddy-Simulation approach

The **parcel model** approach was proven to be accurate up to a threshold of the PR¹ number dependent also from the coarsening factor of the grid.

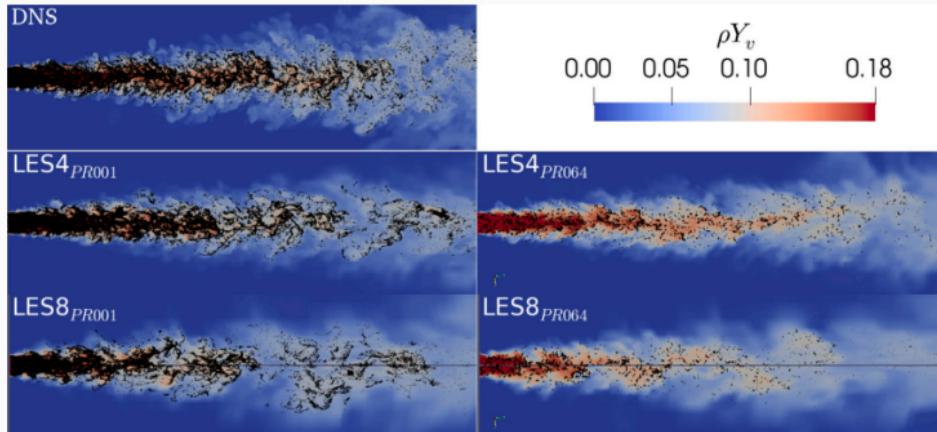


Figure 6: Subset of the simulation runs².

¹PR: Parcel Ratio

²Here the carrier phase is contoured according to the instantaneous vapor mass fraction field (ρY_v)

The research focused on simulating a turbulent diluted acetone jet-spray.

The numerical model was based on:

- LES framework to simulate turbulence behavior
- Hybrid **Eulerian-Lagrangian technique with two-way coupling**
- Parcel model for relaxed droplet tracking

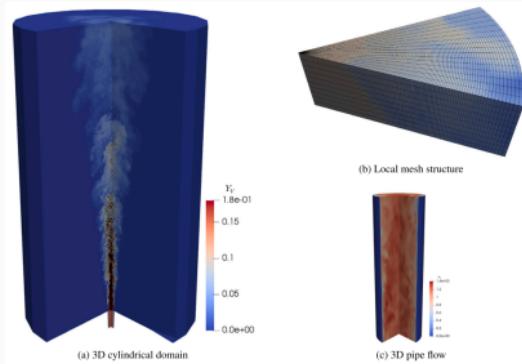


Figure 7: The open-constant pressure-cylindrical domain used for the analysis.

Methodology

Phase 1.1 - Literature Review

A deep literature review to better understand the state of the art in Ammonia combustion and the challenges associated with it will be conducted. We will focus on the following topics:

- Combustion dynamics in ICE¹ (flow engineering).
- Combustion modeling and CFD² simulation for traditional fuels.
- Advanced and optimized algorithms for numerical simulation of a two-phase dispersed turbulent flow.
- Pollution and emissions from Ammonia derivative combustion products.

For our research, we will use ScienceDirect, Scopus, IEEE Xplore as main databases.

A non-exhaustive list of applicable keywords: *Ammonia, Combustion, two-phase dispersed turbulent flow, flash-boiling condition, ICE, CFD*.

¹ICE: Internal Combustion Engine

²CFD: Computational Fluid Dynamics

Phase 1.2 - Model Development

An **accurate and reliable model for Ammonia dynamics (non-reactive)** will be developed starting from previous knowledge of the literature review and experimental data founds.

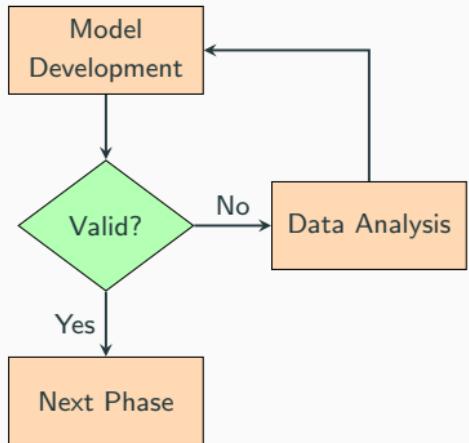
From a first analysis of the physics of the problem, we can expect our CFD model to be based on:

- An **Eulerian algorithm** dedicated to **advance in time the flow fields** by solving the Low-Mach number formulations of the Navier-Stokes equations
- A **Lagrangian solver** designed to synchronously **evolve the mass, momentum, and temperature equations** of dispersed droplets under point-particle approximation.

The model will be developed in OpenFOAM and Chemkin.

Phase 1.3 - Model Validation

The model will be **validated using experimental data** from the literature.



Evaluation test cases are dependent on the literature review and the experimental data founds.

If available, the following metrics will be adopted:

- Droplet size distribution.
- Temperature and pressure profiles.
- Spray geometry (angle, penetration, and shape).

Phase 2.1 - Experimental Campaign

In the optic of gathering as many data as possible, an **experimental campaign with some preexisting injector in the context of Ammonia combustion in ICE** will be conducted.

Main goal: better understand the combustion process of Ammonia in an ICE (**reactive environment**).

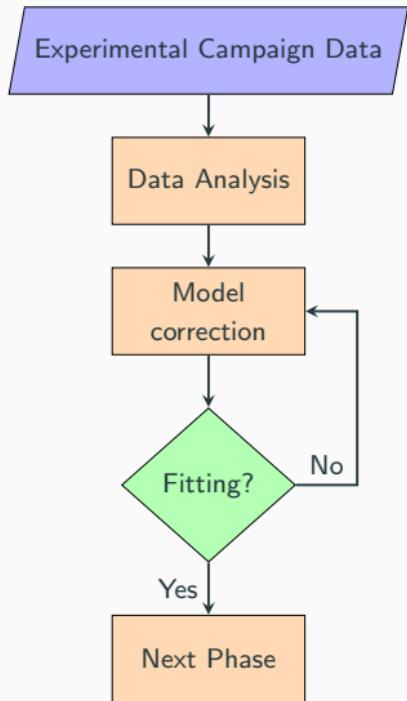
Possible instruments to be used:

- High-speed camera.
- Pressure and temperature sensors.
- Gas analyzer.



Figure 8: Delavan hollow cone nozzle that may be adopted.

Phase 2.2 - Data Analysis



For each experimental test, data will be collected and analyzed.

The following analysis methods might be exploited:

- Data visualization.
- Machine learning.
- Statistical analysis.

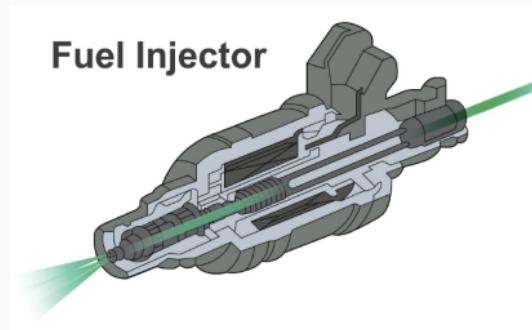
Phase 3 - Fuel Injector Design & Testing

After the final model validation, the **design of the new injector** will follow.

As the CAD system, CATIA V5 will be used.

The key factors driving our design will be:

- Stable flame inside the combustion chamber
- Low-to-zero NO_x emissions



The new design will be **tested in a real ICE** and the data collected will be used **to evaluate its performance**.

Expected Results

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To summarize, the expected results of this research are:

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- Phase 1: Numerical model of the Ammonia dynamics for non-reactive condition.

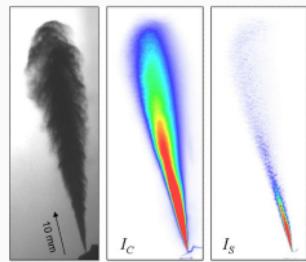


Figure 9: NM¹
(non-reactive condition).

¹NM: Numerical Model.

Expected Results

To summarize, the expected results of this research are:

- Phase 1: Numerical model of the Ammonia dynamics for non-reactive condition.
- Phase 2: Set of experimental data and **numerical model of the Ammonia dynamics for reactive condition**.

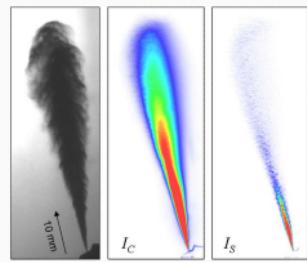


Figure 9: NM¹
(non-reactive condition).

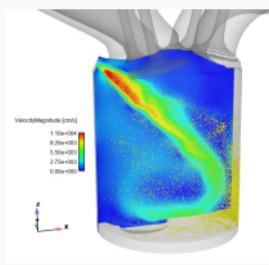


Figure 10: NM¹ (reactive
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Expected Results

To summarize, the expected results of this research are:

- Phase 1: Numerical model of the Ammonia dynamics for non-reactive condition.
- Phase 2: Set of experimental data and numerical model of the Ammonia dynamics for reactive condition.
- Phase 3: **Fuel injector design for pure Ammonia combustion.**

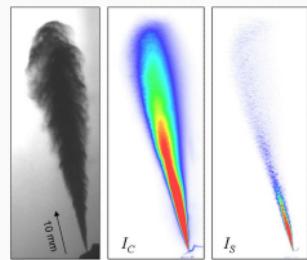


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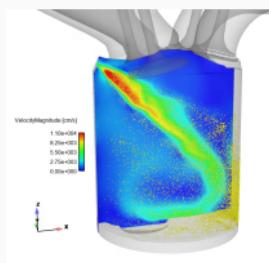


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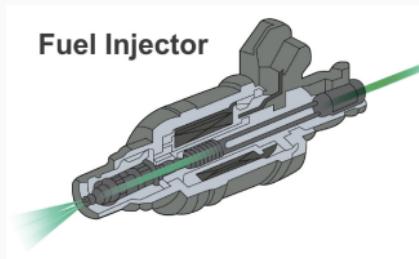


Figure 11: Fuel injector design.

¹NM: Numerical Model.

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Questions?

Thank you!