Designing a Suitable Fuel Injector for Ammonia Using CFD

Next-Generation Fuel in Internal Combustion Engine

Tommaso Bocchietti

March 20, 2024

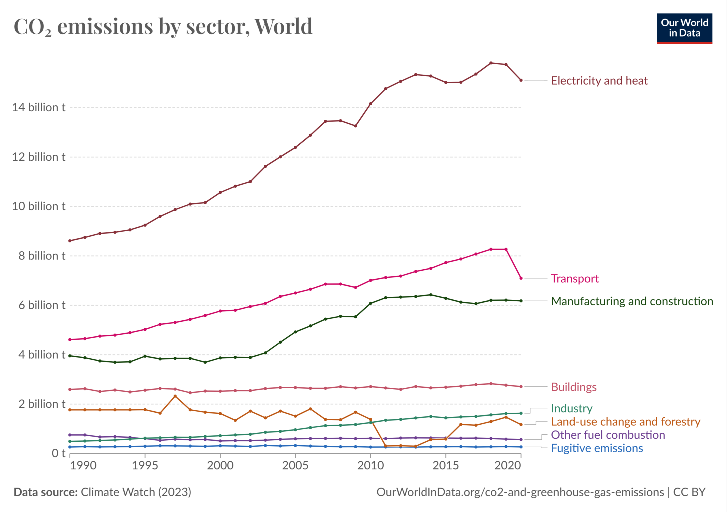
University of Waterloo

Agenda

1. Motivations
2. Research Focus
3. Prior Studies
4. Methodology
5. Expected Results

Motivations

Transportation sector is the second-largest contributor to CO_2 emission.



Transportation sector has been looking for alternative fuels to reduce CO_2 emission.

- **Electricity:** requires a large infrastructure to support the global demand
- **Methane:** worse than CO_2 in terms of greenhouse effect (short-term)
- **Hydrogen:** difficult to store and transport

Researchers started looking at Ammonia as a potential alternative fuel.

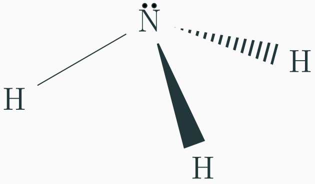


Figure 1: Ammonia molecule (NH_3)

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 NFPAs[1]):

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

[1] National 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 $\mathrm{NO_x}$ emissions

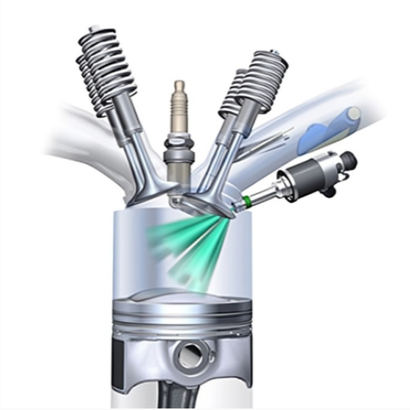


Figure 2: Direct fuel injection in internal combustion engines

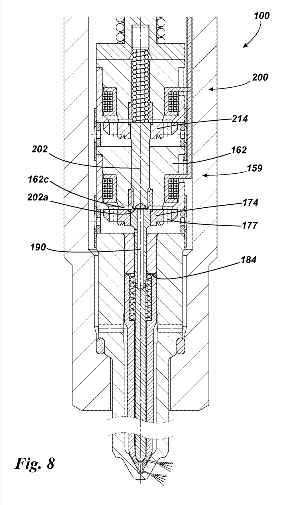


Figure 3: "Fuel injector" (US20120080011A1)

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

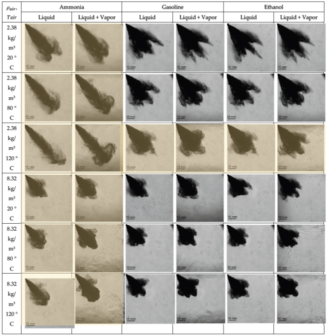


Figure 4: Comparison of spray shape (different fuels & conditions).

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 $\mathrm{LNH_3}$[1] combustion was developed and validated (LES[2] based). Particular attention to the **flash-boiling condition** modelling was given.

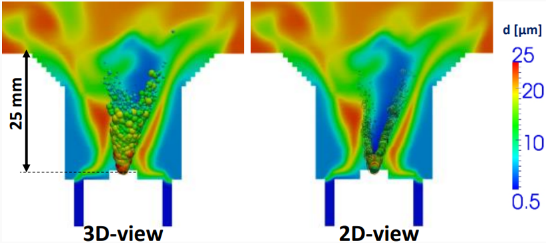


Figure 5: 3D and 2D views of $\mathrm{LNH_3}$ droplet distributions.

[1] LNH3: Liquid Ammonia
[2] LES: 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 PR[1] number dependent also from the coarsening factor of the grid.

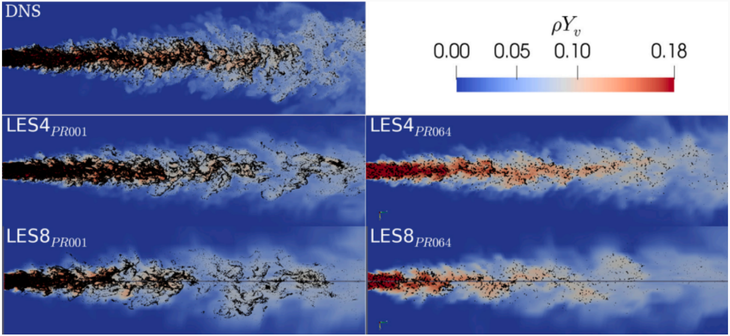


Figure 6: Subset of the simulation runs[2].

[1] PR: Parcel Ratio

[2] Here 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

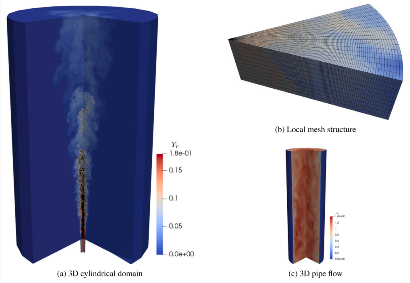


Figure 7: The open-constant pressure-cylindrical domain used for the analysis.

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 ICE[1] (flow engineering).
- Combustion modeling and CFD[2] simulation for traditional fuels.
- Advanced and **optimized algorithms for numerical simulation of a two-phase dispersed turbulent flow**.
- Pollution and emissions from Ammonia derivate 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*.

[1] ICE: Internal Combustion Engine
[2] CFD: 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.

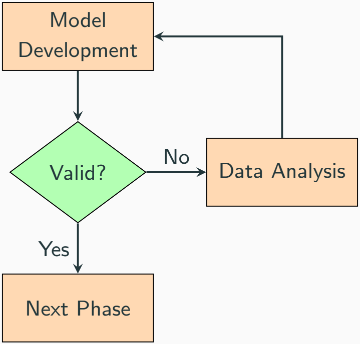
From a first analysis of the physics of the problem, we can expect our CFD model to be based on:

- 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).

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.

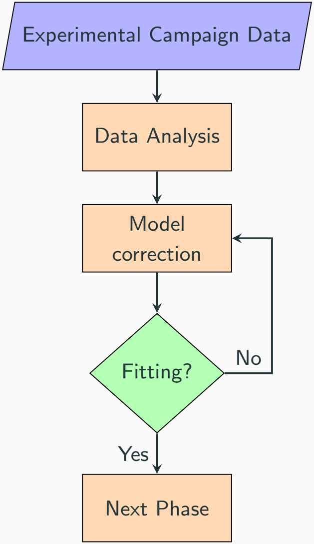
Main goal: better understand the combustion process of Ammonia in an ICE (**reactive environment**).

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.

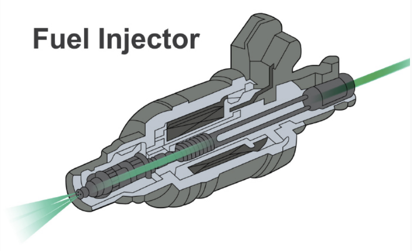
Phase 3 - Fuel Injector Design & Testing

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 $\mathrm{NO_x}$ 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:

[1] NM: Numerical Model.

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

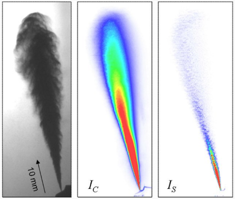


Figure 9: NM[1] (non-reactive condition).

[1] NM: 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**.

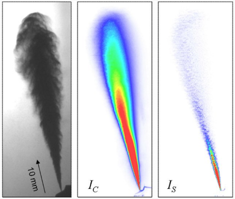


Figure 9: NM[1] (non-reactive condition).

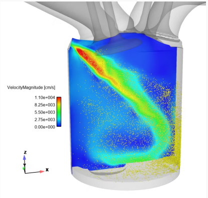


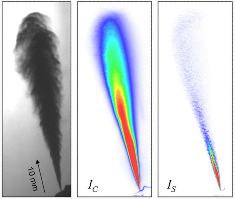
Figure 10: NM[1] (reactive condition).

[1]NM: 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.
- Phase 3: **Fuel injector design for pure Ammonia combustion**.



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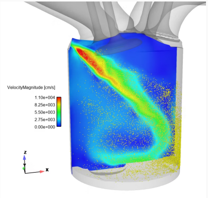

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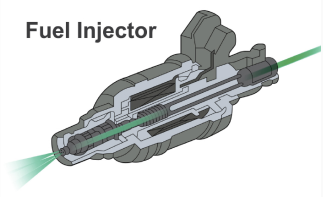

Figure 11: Fuel injector design.

[1]NM: Numerical Model.

Extra slides

NO_x emissions are a family of nitrogen oxides that are commonly associated with combustion processes of Ammonia.

The key factors to reduce the NO_x emissions are combustion temperature and air-to-fuel ratio.

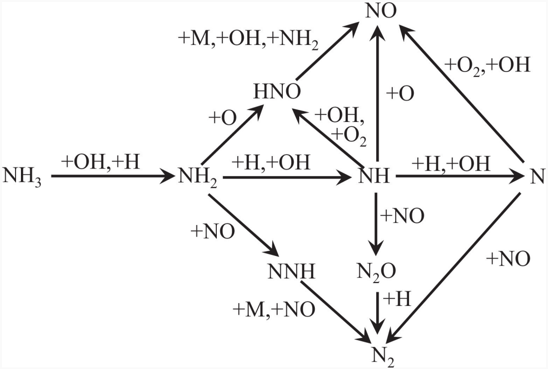

Figure 12: NH_3 oxidation pathway.

Lagrangian approach consists in **following droplets during their movement**.

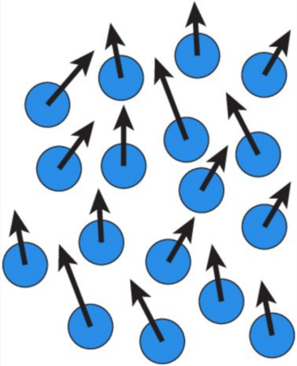

Figure 13: Lagrangian approach.

Eulerian approach consists in **considering inlet and outlet flux in a given volume**.

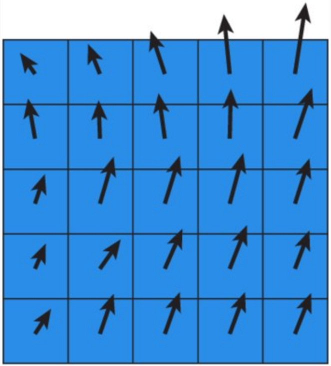

Figure 14: Eulerian approach.

Ansys — engineering simulation software.
https://www.ansys.com/.

Delavan — the global leader in high-quality spray nozzles and fluid handling systems.
https://delavan.com/.

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Questions?

Thank you!