



Written on 28 March 2023



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For transport segments where electrification is complex, such as heavy-duty vehicles (long-haul trucks and off-road<sup>1</sup> vehicles), hydrogen mobility appears to be a promising alternative to address the challenges of reducing the carbon footprint of the transport sector as a whole.

**While fuel cells have been the focus of a substantial amount of research in the context of low-carbon mobility, the IC engine using hydrogen as a fuel appears to be equally feasible as an alternative in order to significantly reduce CO<sub>2</sub> and pollutant emissions. This has been demonstrated by research conducted by IFPEN, FEV and Aachen University as part of the European LONGRUN project.**

To use hydrogen as a fuel, the main challenge is to ensure **a high level of efficiency** while controlling **NO<sub>x</sub> emissions** and **abnormal combustion**. In order to identify the optimization levers for this energy conversion system and gain a better understanding of the phenomena at play, IFPEN partnered up with **FEV** and Aachen University to conduct an experimental and numerical study [1] within the framework of the European **LONGRUN** project.

## **Validation of a 3D approach dedicated to the hydrogen engine**

IFPEN's expertise in the field of reactive CFD<sup>2</sup> modeling and simulation was employed to formulate **a first multi-physical 3D numerical approach** to predict **the behavior of an H<sub>2</sub> engine**.

The simulation is based on a RANS<sup>3</sup> formalization, implemented in the CONVERGE<sup>TM</sup> calculation code, and involves the combined use of **several physical sub-models**:

- The **Extended Coherent Flame Model (ECFM)** [2] which describes the propagation of a partially pre-mixed H<sub>2</sub> flame;
- **The Tabulated Kinetics of Ignition (TKI) model** [3] for the prediction of phenomena related to self-ignition (pre-ignition and knocking);
- and **the detailed post-flame chemical model** (activated only in the burned gas zone) for the prediction of NO<sub>x</sub> emissions.

The modeling approach was validated using experimental measurements provided by FEV and Aachen University for a single-cylinder Diesel engine specifically converted to H<sub>2</sub> for the LONGRUN project.

**The validation of the numerical model** was initially conducted on **a homogeneous PFI<sup>4</sup> configuration** to avoid uncertainties associated with modeling the Air/H<sub>2</sub> mixture in the combustion chamber.

Figure 1 details this validation, which related, in particular, to **the prediction of flame propagation, abnormal combustion phenomena (knocking) and NO<sub>x</sub> emissions**.

<sup>1</sup> Off-road: Any type of vehicle capable of being driven on and off a paved or gravel surface

<sup>2</sup> CFD: Computational Fluid Dynamics

<sup>3</sup> RANS: Reynolds-Averaged Navier-Stokes

<sup>4</sup> PFI: Port Fuel Injection

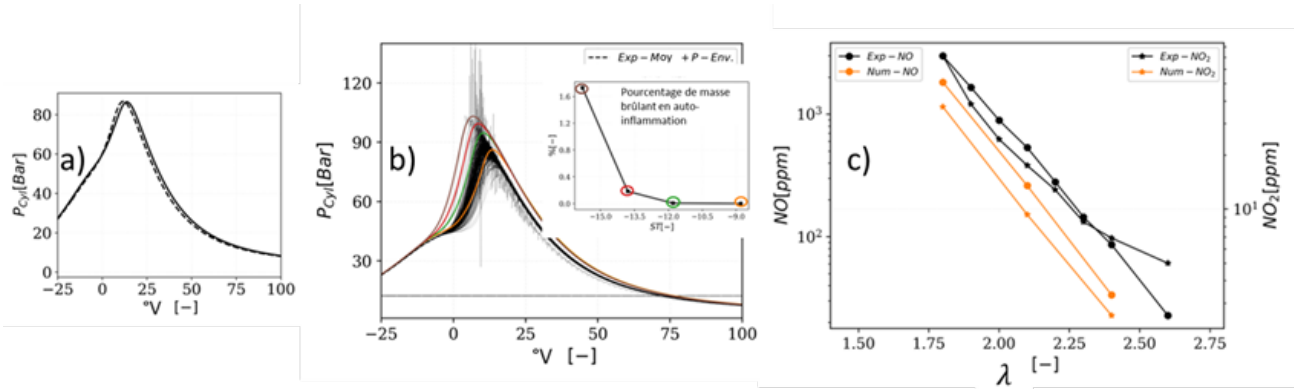


Figure 1. PFI configuration: a) pressure of the numerical cylinder (solid line) compared to the experimental signal (dotted line), as a function of the crank rotation angle; b) experimental pressure envelope on a knock point compared to the numerical envelope obtained for different spark timing (ST) advance values while monitoring the percentage of the H<sub>2</sub> mass consumed during self-ignition; c) comparison between experimental and numerical NO and NO<sub>2</sub> engine exhaust emissions for several values of  $\lambda$ .

The CFD model previously validated for the PFI configuration was then used to simulate a **configuration with direct H<sub>2</sub> injection**.

While reproducing the good evolution of cylinder pressure (and thus flame propagation) compared to measurements, the calculation made it possible to demonstrate that **the optimization of mixture formation on a direct injection (DI) configuration** is a key lever for improving engine efficiency and reducing NO<sub>x</sub> emissions.

Figure 2 shows that NO and NO<sub>2</sub> formation is closely associated with the mixture preparation described by the variable  $\lambda$ <sup>5</sup>. Moreover, this first validation confirmed **the relevance of 3D calculation** as a tool to facilitate and support the design of future hydrogen powertrains.

<sup>5</sup> Air/Fuel ratio

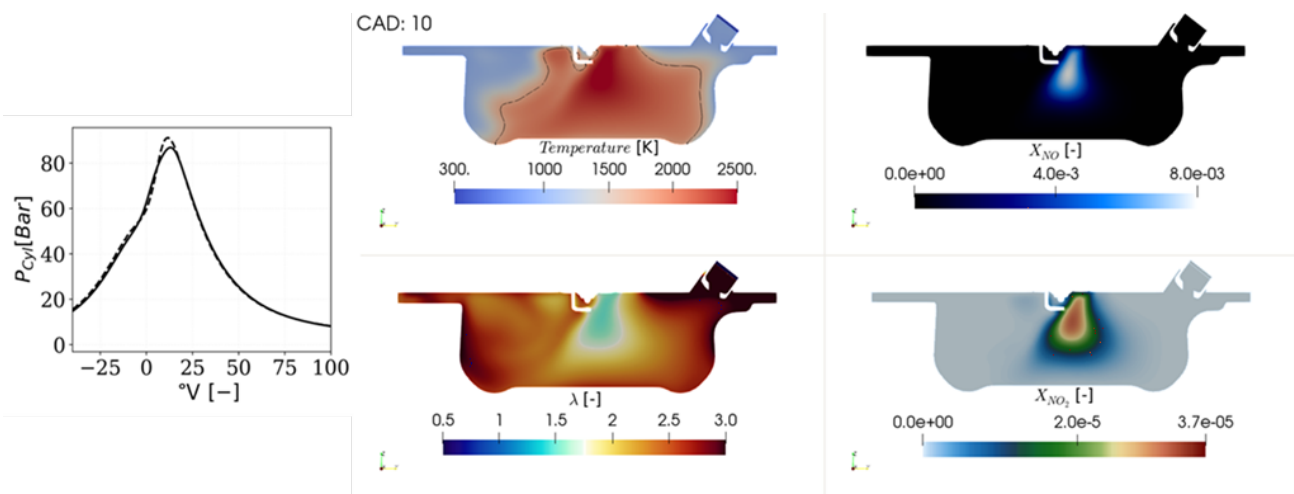


Figure 2. Left: evolution of cylinder pressure on a direct injection point for numerical calculation (solid line) and experiments (dotted line). Right: 2D distribution, on the median plane of the cylinder, of temperature, ( $\lambda$ ) and NO<sub>x</sub> (NO and NO<sub>2</sub>) on a direct injection (DI) operating point with a crank angle degree (CAD) of 10°.

**Ongoing research to improve the predictive capacity of 3D simulation**

The promising results obtained during this research encourage further studies involving new simulation approaches in order to continue to improve **the robustness and predictive capacity of calculations** over a broader operating range (regime and load).

In particular, this research will consist in improving the modeling of the H<sub>2</sub>/air mixture in the combustion chamber during direct injection, as well as the description of flame propagation and the self-ignition phenomenon.

## References

[1] Maio, G., Boberic, A., Giarracca, L., Aubagnac-Karkar, D., Colin, O., Duffour, F., ... & Pischinger, S. (2022). Experimental and numerical investigation of a direct injection spark ignition hydrogen engine for heavy-duty applications. *International Journal of Hydrogen Energy*, 47(67), 29069-29084.

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[3] Robert, A., Richard, S., Colin, O., Martinez, L., & De Francqueville, L. (2015). LES prediction and analysis of knocking combustion in a spark ignition engine. *Proceedings of the Combustion Institute*, 35(3), 2941-2948.

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