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News

Fundamental Research

IC powertrains

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Systems modeling and simulation

For transport segments where electrification is complex, such as heavy-duty vehicles (long-haul trucks and off-road¹ 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 CO₂ 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 **NOx 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 CFD² modeling and simulation was employed to formulate a **first multi-physical 3D numerical approach** to predict **the behavior of an H₂ engine**.

The simulation is based on a RANS³ formalization, implemented in the CONVERGETM 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 H₂ 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_x emissions.

The modeling approach was validated using experimental measurements provided by FEV and Aachen University for a single-cylinder Diesel engine specifically converted to H₂ for the LONGRUN project.

The validation of the numerical model was initially conducted on a **homogeneous PFI⁴ configuration** to avoid uncertainties associated with modeling the Air/H₂ 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_x emissions**.

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

² CFD: Computational Fluid Dynamics

³ RANS: Reynolds-Averaged Navier-Stokes

⁴ PFI: Port Fuel Injection

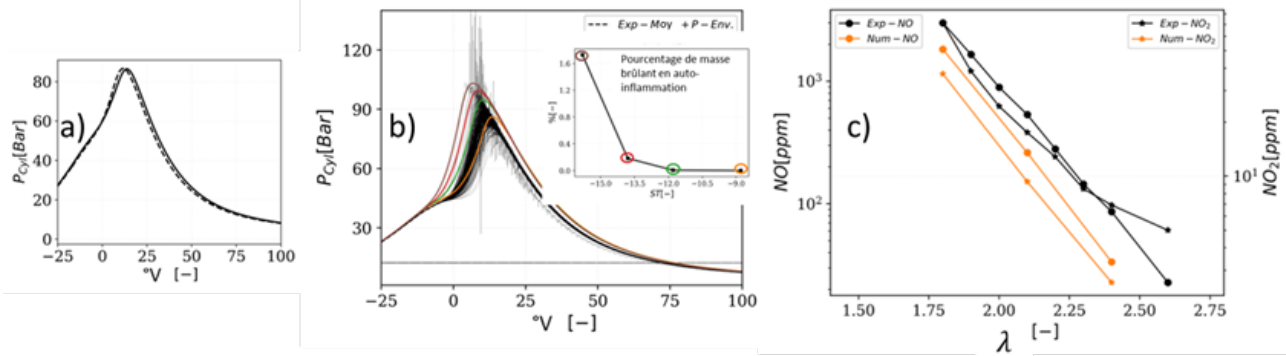


Figure 1. PFI configuration: a) pressure of the numerical cylinder (solid line) compared to the experimental signal (dotted line), as a function of the crank rotation angle; b) experimental pressure envelope on a knock point compared to the numerical envelope obtained for different spark timing (ST) advance values while monitoring the percentage of the H₂ mass consumed during self-ignition; c) comparison between experimental and numerical NO and NO₂ engine exhaust emissions for several values of $λ$.

The CFD model previously validated for the PFI configuration was then used to simulate a **configuration with direct H₂ 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_x emissions**.

Figure 2 shows that NO and NO₂ formation is closely associated with the mixture preparation described by the variable $λ$ ⁵. Moreover, this first validation confirmed **the relevance of 3D calculation** as a tool to facilitate and support the design of future hydrogen powertrains.

⁵ Air/Fuel ratio

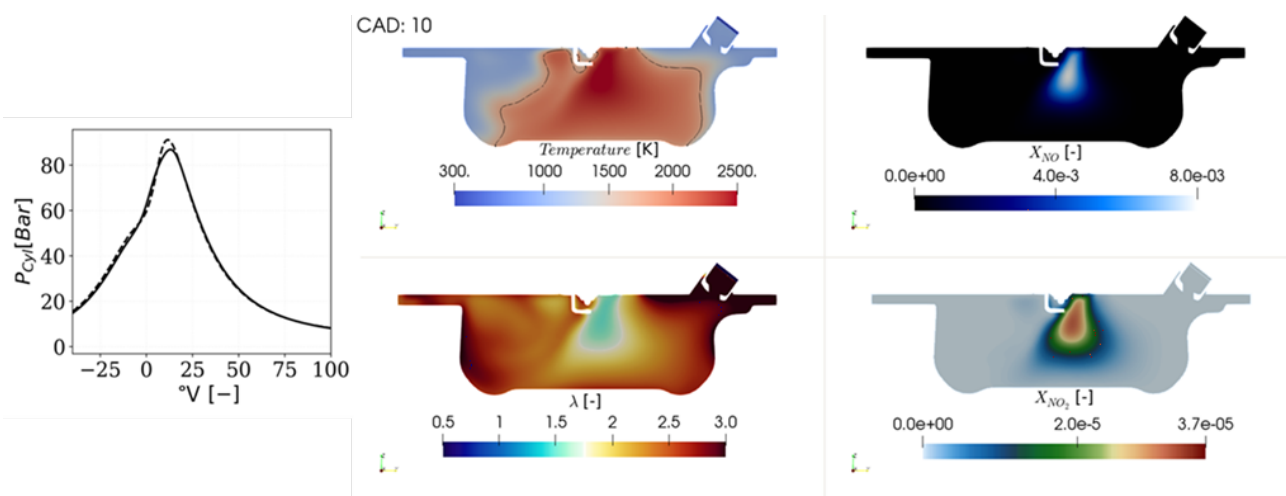


Figure 2. Left: evolution of cylinder pressure on a direct injection point for numerical calculation (solid line) and experiments (dotted line). Right: 2D distribution, on the median plane of the cylinder, of temperature, ($λ$) and NO_x (NO and NO₂) on a direct injection (DI) operating point with a crank 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 H₂/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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