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News

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For transport segments where electrification is complex, such as heavy-duty vehicles (long-haul trucks and off-road[1] 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_2 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 CFD[2] 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 RANS[3] formalization, implemented in the CONVERGE™ 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 H_2 for the LONGRUN project.
The validation of the numerical model was initially conducted on **a homogeneous PFI[4] 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

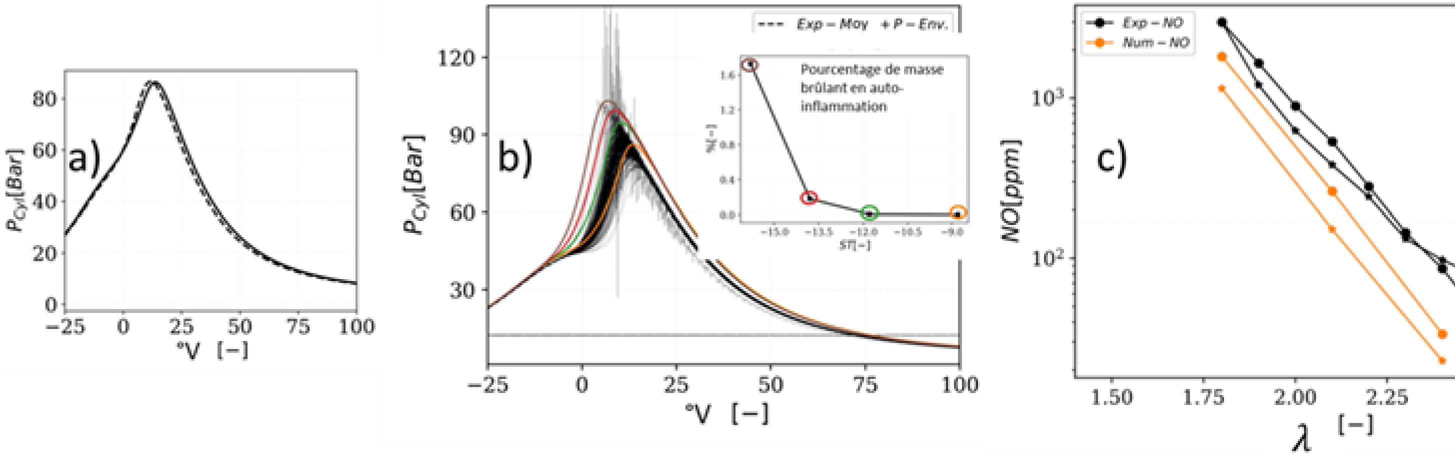

Figure 1. PFI configuration: a) pressure of the numerical cylinder (solid line) compared to the experimental signal (dotted line), as a function of the crank rotation angle; b) experimental pressure envelope on a knock point compared to the numerical envelope obtained for different spark timing (ST) 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 ?.

The CFD model previously validated for the PFI configuration was then used to simulate **a configuration with direct H_2 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 NO_2 formation is closely associated with the mixture preparation described by the variable ?[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

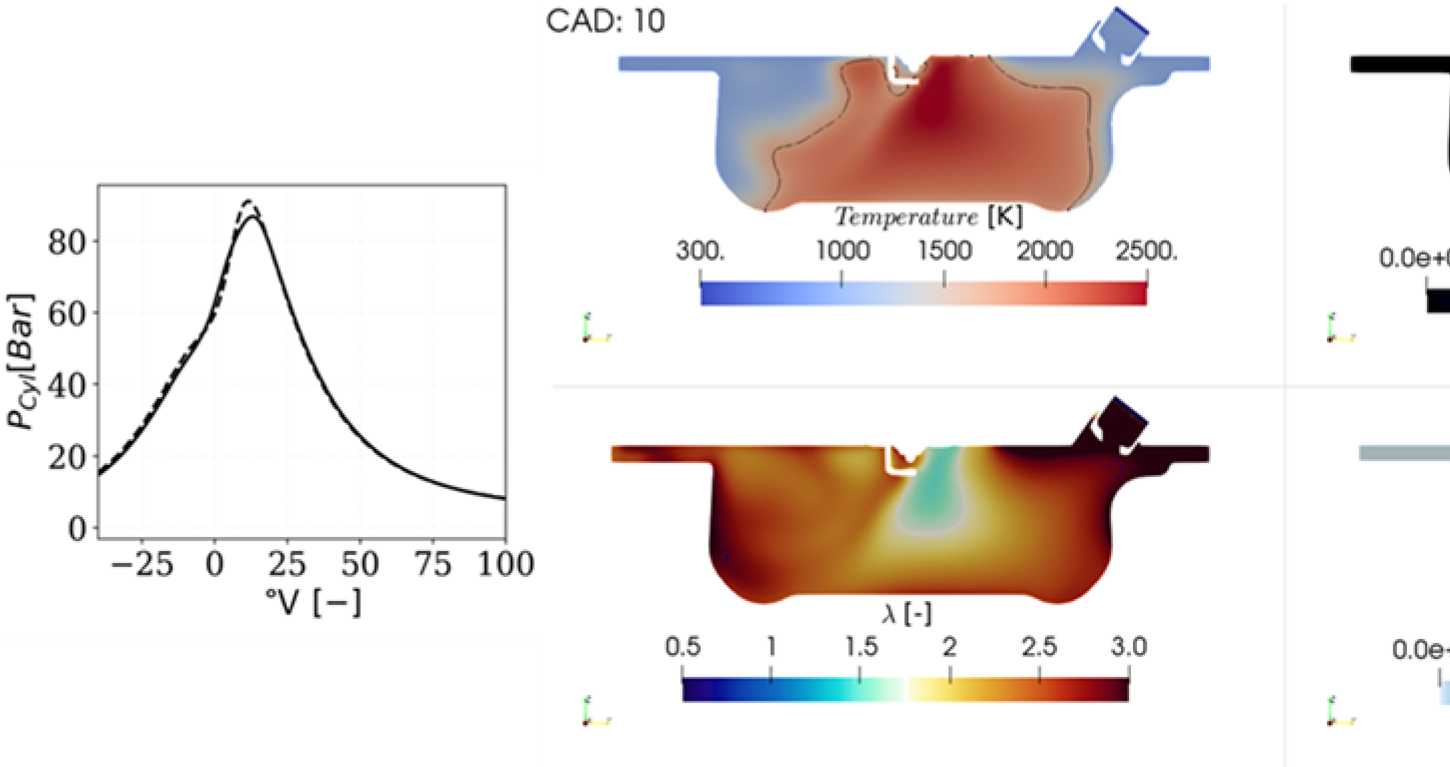

Figure 2. Left: evolution of cylinder pressure on a direct injection point for numerical calculation (solid line) and experiments (dotted line). Right: 2D distribution, on the median plane of the cylinder, of temperature, (?) and NOx (NO and NO2) on a direct injection (DI) operating point with a crank 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 H_2/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.

[2] Colin, O., Benkenida, A., & Angelberger, C. (2003). 3D modeling of mixing, ignition and combustion phenomena in highly stratified gasoline engines. Oil & gas science and technology, 58(1), 47-62.

[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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