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News

Fundamental Research

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The mobility of goods and people is a key component in the development of modern societies, and ensuring its sustainability requires reducing the associated energy consumption while limiting its impact on the environment and health. Developing technological solutions for a **more sustainable** and **socially acceptable mobility** is one of the *raisons d'être* and the driving force of the "Mobility & Systems" Division.

To this end, we contribute to the development of innovative powertrain systems, whether electric, based on internal combustion or hybrid, for low-carbon, energy-efficient mobility with low or zero emissions. Our technological R&I is based on a rich fundamental foundation, combining the development of methods and tools for the design of complex mechatronic systems, simulation techniques and software ranging from system-level to multidimensional, and advanced measurement techniques and equipment. Our points of differentiation stem from our ability to implement them in a design approach that is equally multi-physics (solid and fluid mechanics, thermodynamics, chemical kinetics, electromagnetism), multi-scale (from component to system) and multi-objective (energy efficiency, emissions reduction, mechanical, thermal and chemical strength and durability).

The field of mobility, until very recently focused on fossil-fuel-powered internal combustion engines, has undergone a profound transformation, the scope of which is still difficult to grasp. As such, while electrification will undoubtedly represent one of the major mobility solutions, it seems established that it alone will not be able to meet the complex challenges of mobility, and that complementary approaches based on the consumption of decarbonated fuels and energies will therefore be part of the scope of solutions.

To keep pace with these changes, our Research Division has launched a profound evolution of its research themes. In this context, our originality lies in our ability to invest in electrification-related domains, while at the same time developing our historical focus on combustion and effluent after-treatment, thereby enabling us to offer an innovative and differentiating approach in a highly competitive field.

This special issue illustrates how some of our fundamental research activities feed into and enrich our R&I work in the service of sustainable mobility. We hope that it will bring to light the major changes that have taken place within the “Mobility and Systems” Division, and we invite you to get in touch with the colleagues who will share with you our ambitions for the short, medium and long terms.

LES BRÈVES

The goal of carbon neutrality by 2050 requires a drastic reduction of transport-related CO_2 emissions, which alone account for over 30% of global CO_2 emissions. For road transport, decarbonization is expected to be partly based on the roll-out of battery-powered electric vehicles. However, the constraints imposed by this solution (battery weight and volume, range, charging time, recharging infrastructure) are such that not all uses can be addressed. This is the case for so-called heavy-duty applications (long-haul trucks, coaches, construction equipment), for which carbon-free hydrogen represents a credible alternative.

Two different approaches co-exist and are currently being studied at IFPEN:

- **the internal combustion engine** (ICE), using hydrogen directly as a fuel instead of the hydrocarbons currently available;
- **fuel cells** (FC), which use hydrogen to produce electricity on board and to power a vehicle's electric motor.

The hydrogen internal combustion engine (ICE)

The physico-chemical characteristics of hydrogen and their resulting properties make it a suitable candidate for combustion in an engine: wide flammability range, low ignition energy, high combustion speed.

In 2020, IFPEN began its work with an initial experimental campaign on a single-cylinder engine, which identified the obstacles to be overcome for this type of engine. To use hydrogen as a fuel, one of the main challenges is to ensure a high level of efficiency while controlling NOx emissions, while preventing abnormal combustion that could damage the engine [1] [2]. Figure 1 summarizes the challenges and the IFPEN[1] research avenues for meeting them.

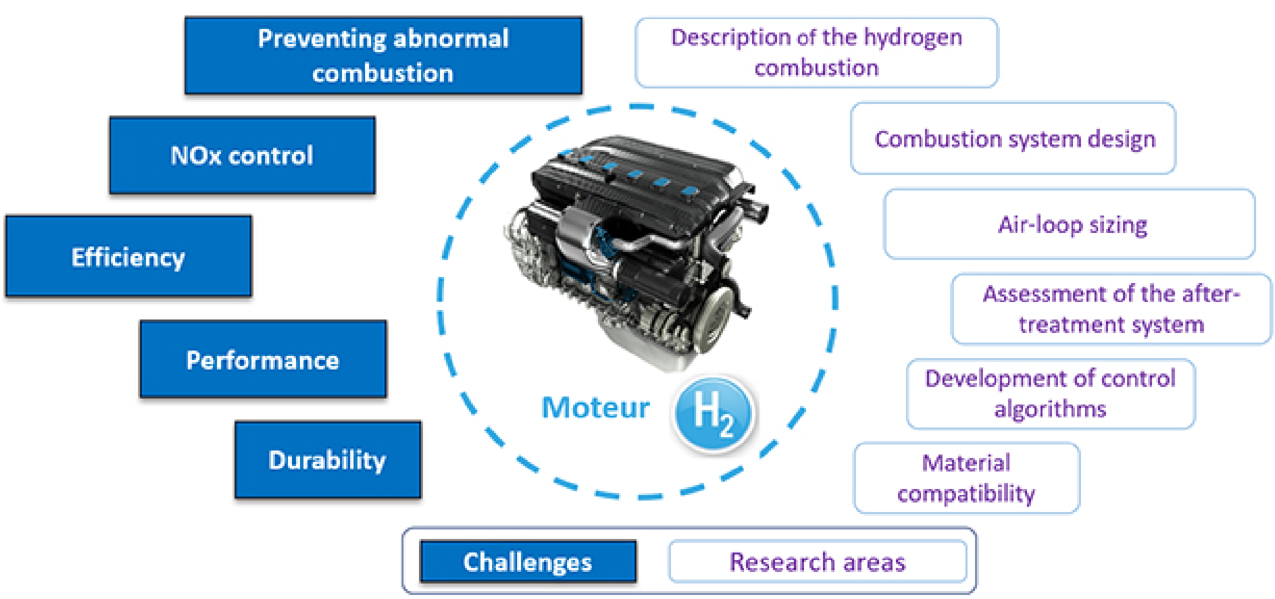

Figure 1: Challenges for the use of hydrogen in internal combustion engines and IFPEN research priorities

Today, IFPEN is committed to developing its resources and skills in order to meet all of the identified challenges [3].

In particular, 3D CFD tools serve to simulate the turbulent hydrogen combustion in an internal combustion engine, so that promising combustion chamber geometries can be optimised as early as possible in the design phase.

Fundamental research is therefore underway to ensure the robustness and predictability of these digital tools:

- visualization and simulation of H_2 injection (figure 2) using advanced visualization tools developed by the "Mobility and Systems" Division;
- simulation using the **Converge code** of the H_2/air mixture in the combustion chamber during direct H_2 injection (figure 3);
- description of flame propagation and auto-ignition, representation of parietal phenomena[2].

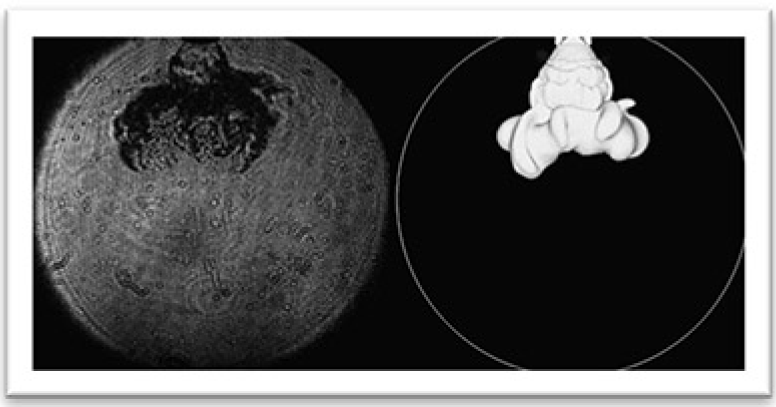

Figure 2: Visualization and simulation of H2 injection in a cell

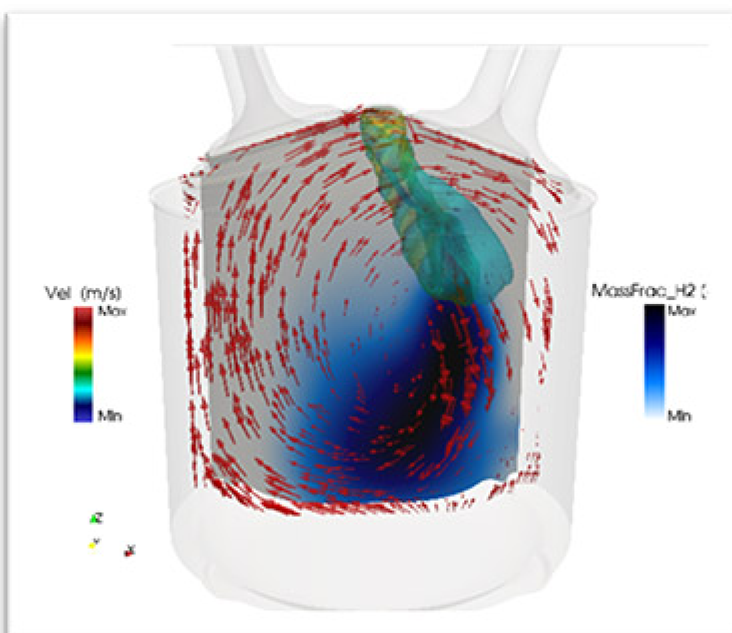

Figure 3: Simulation of H2/air mixture injection into an engine combustion chamber

Fuel cells (FC)

The fuel cell vehicle is an alternative solution to the all-electric vehicle when the use of a battery alone no longer meets the user's demands: energy requirements exceeding 0.5 MWh profile over a given mission, or intensive use incompatible with a recharging time of several dozen minutes [4, 6].

The use of one or more FCs on board a vehicle requires a "system" approach in order to manage the many interactions between the various functions, both during vehicle design and during use: combined electricity generation (FC and battery), electrical adaptation between sources and on-board consumers, cooling of all vehicle components, consideration of the effects of FC ageing, etc.

The developments of the "Mobility and Systems" Division, carried out in close collaboration with other IFPEN divisions[3], focus on three aspects:

- optimising the sizing of the battery/FC pair in order to consider not only energy requirements, but also power demands during the vehicle's assigned mission [5];
- the design of power electronics adapted to the simultaneous management of several sources of direct current (DC), with varying voltage at any given moment;
- minimizing the ageing of the battery/FC pair, through better identification and consideration of the phenomena that accelerate ageing, and optimising their coupled operation.

With regard to the latter, detailed modelling of the electrochemical and thermal phenomena at the heart of the fuel cells is currently underway (figure 4). The formation of liquid water at the heart of the cell - following the hydrogen reaction - then its transport and finally its evacuation are the subject of a specific study.

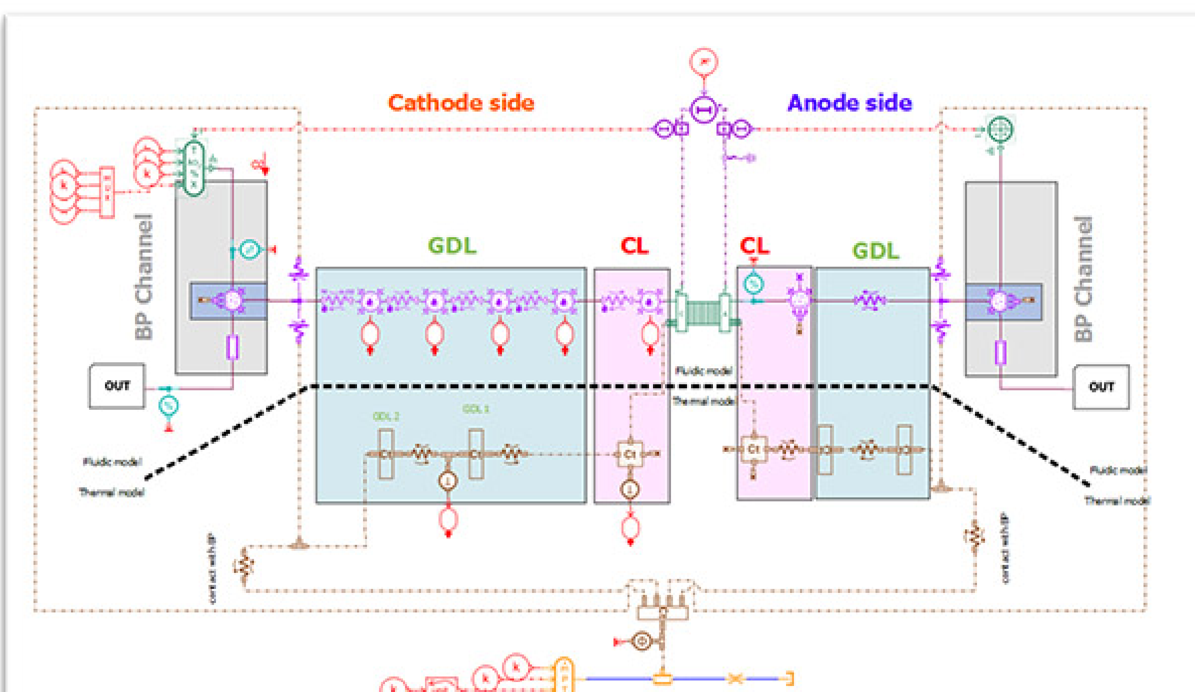

Figure 4: Fuel cell model for detailed consideration of electrochemical and thermal phenomena (Simcentre Amesim® platform)

This detailed analysis of the specific features of these two propulsion modes using hydrogen as an energy vector is intended to provide complementary solutions as quickly as possible, adapted to the various usage cases of carbon-free mobility.

[1-] Each challenge can be addressed by several research axes and vice versa
[2-] Wall-related phenomena: heat transfer, formation of hot spots, etc.
[3-] "Digital sciences and technologies", "Physical chemistry and applied mechanics", "Economics and business intelligence"

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   Video on YouTube – Speech by Pierre Leduc (from 00:36:00 to 01:15:00) :

>> https://www.youtube.com/watch?v=KJBNfNuGQHM

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Hydrogen: two complementary paths to sustainable mobility

By combining battery, electric machine, power electronics and mechanical transmission, the electric vehicle is an example of an application that combines a range of constraints for the formulation of technical fluids.

In recent years, there has been renewed interest in the study of the latter for the transport sector.

This concerns both the formulation of products with low environmental impact and the optimisation of blends to meet complex working conditions.

Indeed, in addition to their lubrication and heat transport functions, their compatibility with materials must be ensured, and the presence of electromagnetic fields requires monitoring of their dielectric properties. Finally, all of this must be done without impairing their lifespan, as required by the specifications.

However, the formulation of these fluids still relies heavily on experimental results that are not easily transposable to the new systems under study. In addition, the combination of different stresses increases the complexity of their alteration mechanisms, and therefore the evolution of their properties in service, thereby requiring new experimental and numerical methods to understand their origins and support technological developments where they are present.

For this reason, IFPEN's teams have launched a research programme to better understand ageing processes in multifunctional environments for the various fluids used in electric vehicles (figure 1). The process is divided into three stages:

- the first aims to assess the response of various fluids to successive stresses, such as measuring the impact of mechanical shear prior to an oxidation process;
- the second is to develop a new experimental device based on microfluidics for coupled characterization of the impact of given stresses (shear, oxidation, electromagnetic field, etc.) on small volumes of fluid;
- the last aims to extend our approaches to the modelling of ageing aspects by combining chemometrics[1] and chemical kinetics, based on understanding at the molecular scale, in order to identify relevant chemical descriptors in order to qualify it.

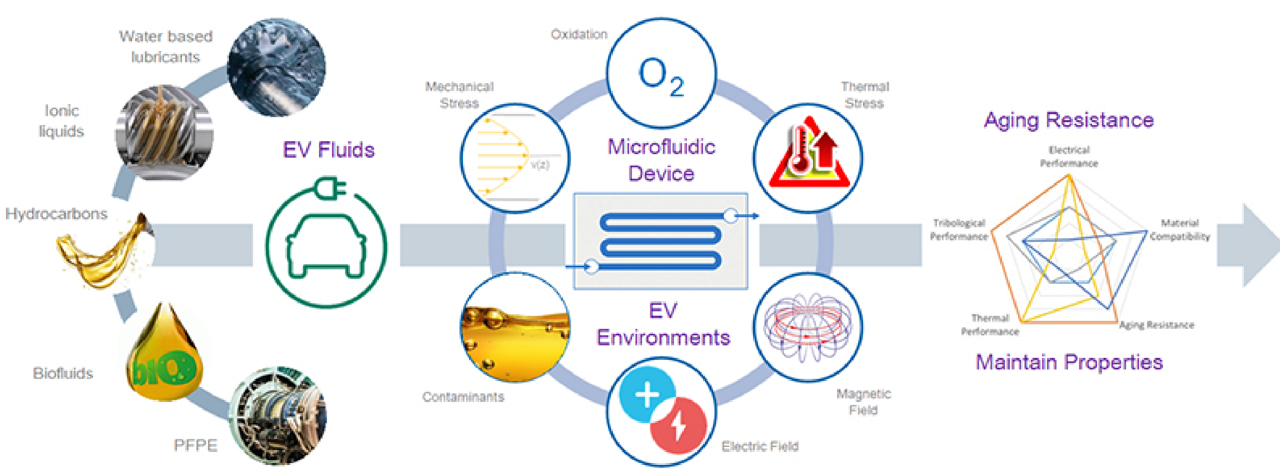

Figure 1: Illustration of the methodology used to study the ageing of technical fluids in complex environments.

IFPEN has also set up a rheometer equipped with various accessories (magnetorheology, electrorheology, gas purging, temperature control) to carry out in-situ and ex-situ measurements of liquid properties in a controlled environment and under multiple stresses. This equipment is currently being used for the first characterizations of technical fluids in complex environments on behalf of a research consortium initiated at the end of 2022 and led by IFPEN. It brings together carmakers and producers of technical fluids that, in addition to assessing their products, hope to push back the limits of their use, with a view to new applications. In parallel, post-doctoral work is evaluating the use of chemometrics in order to characterize the ageing of these fluids on a laboratory scale [1].

The optimised use of technical fluids in transport is both an economic and an environmental challenge that still raises many research questions, which is why IFPEN is involved in both understanding and deploying the associated resources. To overcome the underlying scientific challenges, this research is also part of a collaborative approach with academic laboratories.

[1-] Chemometrics is the application of mathematical tools, particularly statistical ones, to obtain maximum information from chemical data.

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Ageing of technical fluids in multifunctional environments

According to the WHO, 7 million premature deaths worldwide each year are linked to poor air quality, a problem to which road transport makes a significant contribution. Thanks to regulatory and technological developments, as well as the renewal of the vehicle fleet, emissions from this sector have certainly been falling in recent years. However, it remains a major contributor to the deterioration of air quality, with, for example, 49% of NOx emissions in France in 2020 (half of which from private vehicles) and 13% of PM2.5 emissions[1] (1/3 of which from private vehicles).

An assessment of the implemented remediation solutions (vehicle technologies, infrastructures, uses) must be based on a precise, exhaustive and reliable diagnosis of both the sources (raw gases at emission points) and the resulting air quality (diluted gases and generation of secondary pollutants). In addition, air quality can be greatly affected by local conditions (confinement, meteorology, etc.), and vehicle emission levels are highly sensitive to their actual usage conditions. As such, it is crucial to equip ourselves with the tools needed to assess the latter and their impact on pollutant emissions.

In this context, the approach proposed by IFPEN to relate vehicle emissions to actual driving conditions couples:

- on-road measurement;
- vehicle-scale modelling;
- large-scale collection of usage data.

For any geographical area of interest (urban centre, residential, close to traffic, etc.), this approach makes it possible to quantify the variability of emissions in real use as a function of the vehicle fleet and driving behaviour, in order to envisage appropriate remediation solutions.

Design of measurement system

Research work has focused on ultraviolet spectroscopy, culminating in the ELEMENTS multi-gas analysis system [1,2], which measures nitrogen oxides (NOx) among other things, and current developments are exploring its use as a tool for quantifying fine particles.

The development of the chemometric algorithm required the set-up of a digital testing platform in order to simplify the calibration phase.

The developed tool makes it possible to create composite spectra combining information from the literature (reference spectra) and the noise and defects of the actual optical system (light source, spectroscope, optical path). This has served to broaden the range of measurable compounds: combustion indicators O_2, H_2O)[2] and certain industrial pollutants (H_2S, Cl_2, Benzene, Toluene), in addition to the panel of gases already characterized (NO, NO_2, NH_3, SO_2).

Thesis work [3] has also validated the feasibility of exploiting the scattering properties of combustion particles in ultraviolet as a function of their physical and chemical properties.

Roll-out of field measurements

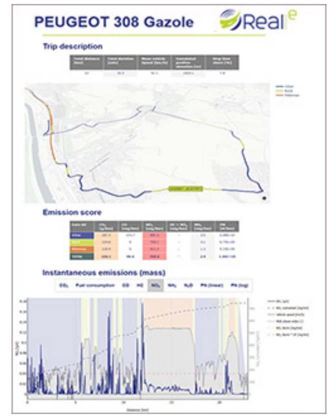
To measure emissions at the heart of road traffic, the ELEMENTS analyser has been integrated into the "RealE" on-board measurement system (see figure 1) [2, 4].

This tool has been used to assess the environmental performance of passenger cars as part of a study for the public authorities. It has made it possible to provide objective data on actual emissions from vehicles meeting the latest emission standards (Euro 6), while also focusing on certain compounds not yet regulated (Euro 7) [5].

The RealE analyser is also at the heart of several studies:

- for Ademe (French Environment and Energy Management Agency), with the aim of assessing the potential of on-board measurement for increased monitoring of vehicle fleet performance [6];
- as part of the European LENS project, dedicated to assessing and reducing emissions from 2-wheelers [7].

Figure 1: Illustrations of the RealE on-board analysis system



These studies under real-life conditions were preceded by extensive laboratory campaigns, for example as part of the RHAPSODIE 1 and 2 studies[3], which made it possible to draft a comprehensive overview of vehicle emissions, both regulated and unregulated, gaseous and particulate[4], while also determining the impact of biofuels introduced at different rates [8].

Extension to vehicle fleets and territories

Working in close synergy with IFPEN's "Digital Science and Technology" division, the "Mobility and Systems" division is carrying out research to model road transport emissions under a variety of real-life conditions, and to derive simulations not just for a given vehicle, but on the scale of the vehicle fleet, across a territory encompassing a multitude of engine technologies and usage cases.

This approach has notably been deployed to assess the relevance of various levels of electrification for the decarbonization of passenger cars [9, 10].

Development of remediation solutions

To limit pollutants at the source, work is being carried out with IFPEN's "Catalysis, Biocatalysis and Separation" division, to find innovative treatment solutions. For example, high-capacity NOx adsorbents based on zeolites have been developed [11].

Compared with the state of the art, the developed zeolites can also be used in selective ammonia reduction (NH_3-SCR), thereby resulting in a gain in terms of reaction initiation temperature and hydrothermal stability of the catalyst [12].

[1]- Particles with diameter ? 2.5 µm.
[2]- Measured in combustion products in order to monitor mixture richness, and also to switch from dry to wet measurement.
[3]- Conducted in connection with the ADEME CORTEA calls for projects (Knowledge and reduction of air pollutant emissions).
[4]- 150 compounds studied, as well as particle number measurement.

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Road transport emissions: integrated research for air quality!

Like all sectors concerned by electrification, the transport sector requires the design of high-performance, efficient electrical systems that respond to multiple constraints, such as cost and compactness. In this context, optimisation has become an essential step in the design process of these systems, particularly for electrical machines.

When designing an electrical machine, methods based on finite elements, recognised for their accuracy and generic nature, are often used to simulate its performance. However, due to their relatively long computation times, the use of these methods in optimisation loops is penalizing, all the more so in the case of stochastic optimisation algorithms which themselves require a large number of computations.

Research work is being carried out within the “Mobility and Systems” Division[1] to propose new optimisation methodologies intended to address this computation time issue. Approaches such as the use of substitution models are already in use [1]. Other approaches, such as Bayesian optimisation[2] and multifidelity optimisation, are also being considered. In addition to reducing computation time, these approaches could lead to more relevant modelling and optimization of the power system under study, by enabling more complete consideration of the physical phenomena governing its behavior.

Once the electrical machine designed, ensuring its correct behavior under all operating conditions involves developing and implementing control laws and diagnostic solutions that will serve to control it in the best possible way.

The global approach developed and used for the control and diagnosis of electrical machines is illustrated in Figure 1.

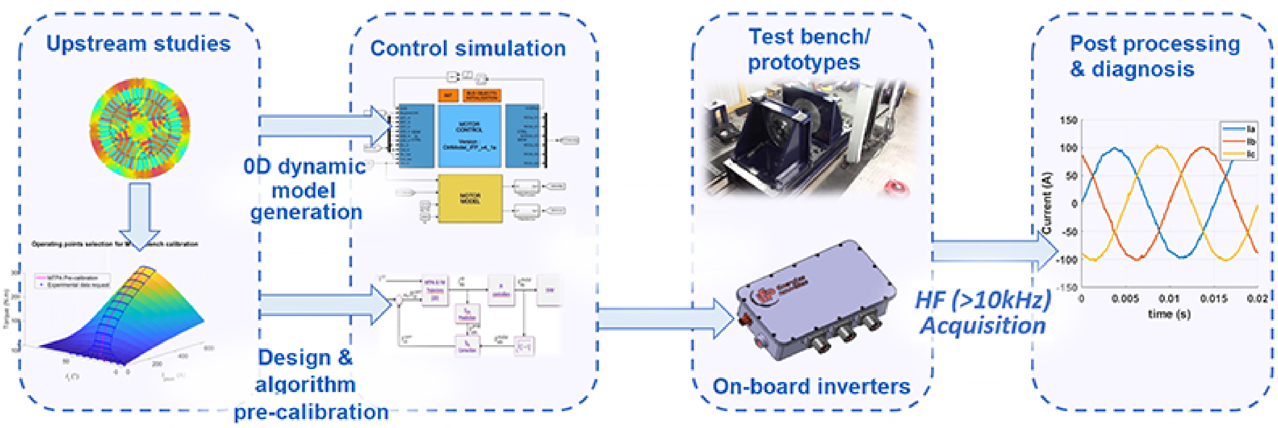

Figure 1: Principle of the global approach to electrical machine testing and diagnosis

In terms of control, dedicated algorithms have been developed within the department to ensure optimum and robust behavior over the entire operating range. These algorithms use design data and an automatic code generation system to speed up the software implementation phase in the inverter control boards also developed by IFPEN.

On the subject of diagnosis, research work is being carried out to develop fault indicators for monitoring the health of stators and rotors:

- In the case of stator monitoring, the idea is to monitor the ageing of the insulation so as to anticipate the appearance of serious inter-turn short-circuit faults. A wavelet transform method has therefore been developed to identify and locate incipient inter-turn defects [2] ;

- In the case of rotor monitoring, the aim is to supervise the magnets, to detect the appearance of demagnetization faults and thus anticipate any drop in the machine performance. A finite element approach has enabled us to develop an indicator of this type of fault by using the zero sequence component of the back electromotive forces [3].

On these two types of defect, a gain in terms of detection sensitivity is expected through a behavioral approach in the high-frequency zone, currently under development. Our work focuses on modelling phenomena and developing dedicated signal processing methods. In addition, to obtain a good compromise between calculation time and accuracy of results, hybrid simulations, combining finite element calculations and based on equivalent electrical circuit models, have been adopted[3].

The modelling, optimization, the control and the diagnosis of electrical machines, carried out by the “Mobility and Systems” division, cover the entire life cycle of electrical machines, from the design phase, through commissioning and performance validation, to monitoring their operation under real-life conditions.

[1-] By the "Electrical and Electronic Systems" division, in collaboration with the "Applied Mathematics" department of the "Digital Science and Technology" division.
[2-] Thesis by Adan Reyes Reyes : *“Contribution méthodologique au dimensionnement optimal et robuste des machines électriques dédiées aux chaines de traction VE et VEH”.*
[3-] Thesis by Jérémy Creux: *“Modélisation hautes fréquences des machines synchrones à aimants, Application à la détection précoce des défauts inter-spires et des défauts de désaimantation”.*

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Electrical machines: Design, optimization, control and diagnosis

In the case of electrified vehicles, whether battery-powered (electric or hybrid) or powered by fuel cells (FC), power electronics (PE) converters play a major role, as they are used for a variety of functions. For example, they are used to drive electric motors, manage on-board energy or control traction battery recharging.

PE refers to an electronic system for converting electrical energy by switching semiconductor transistors, for which silicon (Si) is the historic and still widely used material. But in recent years, the breakthrough of new, more sophisticated transistors, particularly made from materials such as silicon carbide (SiC) and gallium nitride (GaN), has turned the power component market upside down, as their performance surpasses that of their Si-based counterparts.

These new materials, known as "wide band gaps" (WBG[1]) , offer excellent performance in terms of efficiency, power density and switching speed, with a beneficial impact on power losses (figure 1).

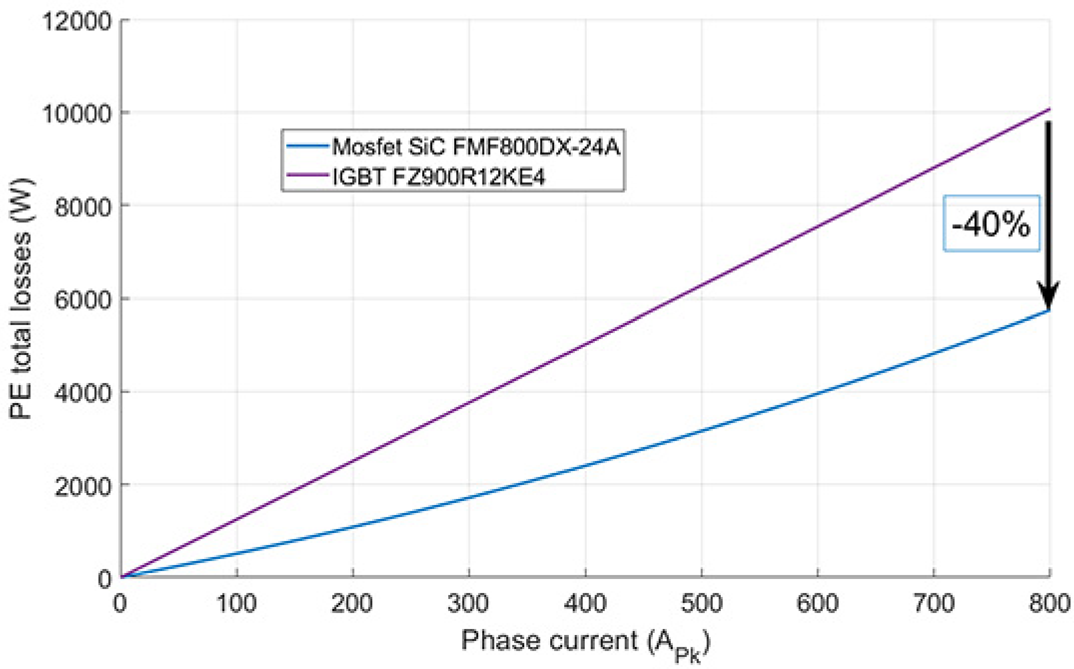

Figure 1: Comparison of losses on a power electronics board with similar silicon carbide (SiC Mosfet) and silicon (IGBT) components at different electric motor current amplitudes.

However, this technological breakthrough brings with it new challenges that the “Mobility & Systems” Division is seeking to meet through research work at a wide range of maturity levels, as part of partnership projects or through doctoral theses.

PE-related research areas include:

- **understanding and characterizing WBG components in a system environment**: this area aims to characterize WBG components with a view to enriching the models used to study them within an electrical system [1]. To this end, IFPEN has entered into a partnership with the company CGD (Cambridge GaN Devices) to understand the impact of implementing these new technologies in converters, and to model the parasitic effects, which can have a major impact on the performance of electrical converters, or even lead to their deterioration. A complementary objective is to develop new test methods dedicated to WBGs, taking into account increasingly severe mission profiles, in order to assess their reliability as well as their fault mechanisms;

- **power converters and innovative topologies**: in this area, IFPEN is involved in the development of new architectures aimed at exploring the efficiency of WBG components to increase the mass and volume power densities of converters and meet increasingly stringent electronic durability requirements. In this context, traction inverter solutions[2] [1] based on silicon carbide (SiC) components have been developed (figure 2). IFPEN is also contributing to research into new power conversion architectures for the hybridization of battery/FC systems [2] in the field of heavy transport, and is involved in the development of prototype solutions for driving electrified compressors that supply air to fuel cells [3] ;

- **thermal management and new cooling solutions**: converters based on Si components are generally cooled indirectly via a "water plate" type heatsink. However, using WBG components to their full potential can generate local power losses of the order of 1 kW/cm^2, i.e. ten times greater than those of Si chips. IFPEN is therefore exploring new localized cooling solutions for the semiconductor chip, while notably focusing on a better understanding of the thermal behaviour of components implemented within electronic boards. The aim is to derive a model capable of better predicting the junction temperatures of WBG components, as these cannot generally be measured directly.

Figure 2: IFPEN traction inverter in SiC technology for automotive applications with a high power density.

All of this ongoing work on PE is aimed at improving the performance and reliability of the energy conversion systems that implement the latest-generation transistors, in order to exploit their full benefits in the context of vehicle electrification.

1- Wide Band Gap.
2- Energy conversion unit that drives the electric motor of an electrified vehicle from a DC voltage source such as the traction battery.

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Power electronics at the heart of electric mobility challenges

The thermal management of electric motors is an essential element in competitive low-carbon mobility, since more efficient cooling not only increases motor performance density (power or torque by mass), but also improves operational reliability by preventing deterioration phenomena (such as demagnetization). Also, oil injection on the most thermally stressed parts (e.g. stator coil heads) appears to be a promising solution for improving the cooling performance.

The development of such systems must be based on optimum design and sizing, which requires detailed knowledge of heat exchange and convection coefficients between the liquid and the components to be cooled. Moreover, the oils used for cooling electrical machines have special properties (high Prandtl number[1]) which lead to large differences between the characteristic scales of flow (> 1/10 mm) and heat (< 1/10 mm), making it difficult to understand the phenomena and predict them using numerical simulations. In addition, the data currently available comes from tests with water-impact jets, and is therefore not representative of the situation currently under consideration.

To overcome this lack of data, a basic experiment with a simplified configuration, in which the oil is sprayed onto a heated flat plate (figure 1a), was developed and carried out to precisely characterize convective heat transfer in this configuration [1]. Surface temperature was recorded using high-precision thermocouples, and advanced optical fluorescence techniques were deployed so as to simultaneously obtain local temperature and oil film thickness. Combining the experimental data obtained with numerical simulation results of heat conduction in the plate made it possible to characterize the overall thermal behaviour, and in particular the local heat flux extracted from the plate (Figure 1b).

This methodology was developed and used in a thesis[2] with the aim of characterizing heat dissipation during the interaction of a liquid jet with a hot plate, as a function of operating conditions (injection rate, oil temperature, etc.). The tests completed in this manner led to the development of empirical correlations between these parameters, which are extremely useful for the design of new electrical machines.

The same methodology will now be applied to cases closer to the application under consideration, such as complex geometries like windings, in order to generate new empirical correlations. These will be essential to the development of reliable and representative models to describe fluid flow and heat exchange in electric motors, while limiting calculation times for design offices.

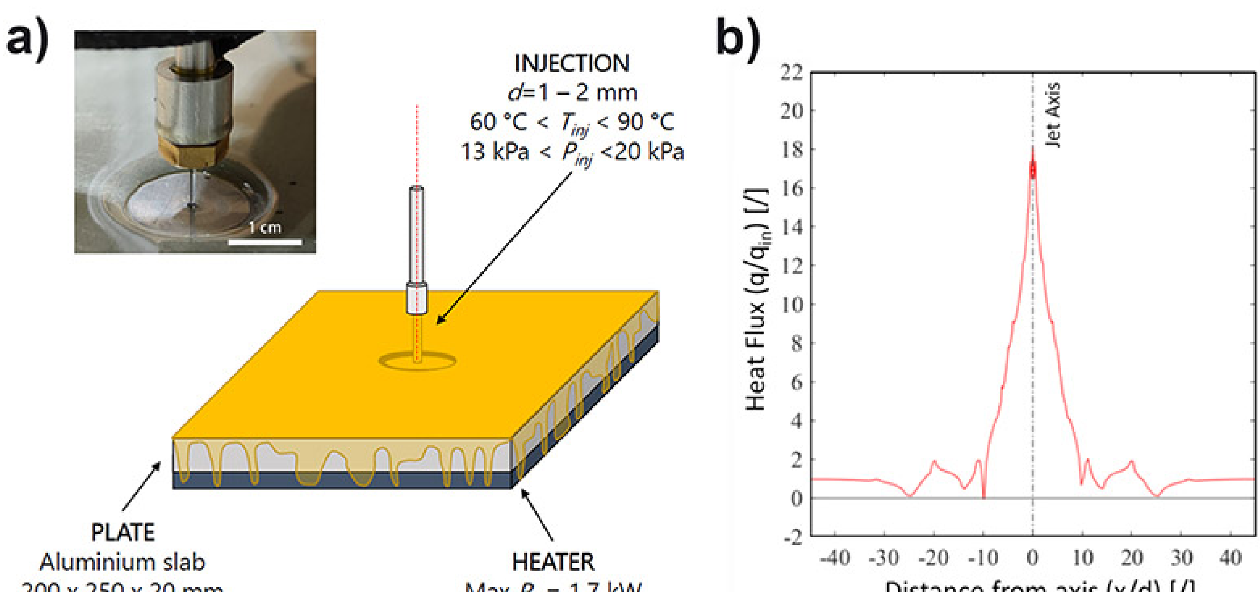

Figure 1: Liquid jet test impacting a hot plate.
1.a Experimental configuration of a liquid jet impacting a hot plate.
1.b Result of the developed methodology, characterization of the heat flux extracted by the impact of the jet on the plate.

1- Dimensionless number, defined as the ratio between kinematic viscosity (related to movement quality) and thermal diffusivity (related to quantity of heat).
2- Entitled *“Développement d'une méthodologie expérimentale pour caractériser les systèmes de refroidissement par liquide des moteurs électriques”*.

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Electric motor: oil cooling is more difficult

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