Science@ifpen

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Transport is a fast-evolving sector: a race to improve efficiency, diversification towards alternative fuels and the demand for partially electrified or all-electric systems are the current driving forces for innovation.

Thanks to the expertise of its researchers and their capacity to tackle new challenges, in collaboration with world-acclaimed academic and leading industry partners, IFPEN is an internationally recognized player in today's transport sector.

The global system approach adopted by IFPEN is based on the development and use of simulation tools, including large-eddy simulation (LES) methods. A recent bibliometric study reveals that IFPEN is the world leader in the field of LES applied to engines. These tools are combined with cutting-edge experimental methods, without ever losing sight of the industrial objectives.

This issue outlines a few significant examples of the work carried out by IFPEN. We hope that you enjoy it.

Stéphane Henriot,
Director of the Energy Applications Techniques Division

Combustion jumps the gun

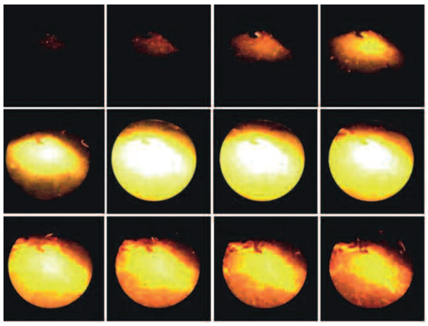
Spark ignition engines operating at high loads are vulnerable to abnormal combustions, limiting their efficiency and jeopardizing their mechanical integrity.

These abnormal combustion phenomena include uncontrolled auto-ignition of the mixture before spark ignition: pre-ignition at low engine speed. The causes of this problem are difficult to identify since numerous interacting factors can adversely affect the local thermodynamic conditions promoting auto-ignition.

Using an experimental and numerical approach, IFPEN has developed an integrative strategy to identify the main mechanisms involved in auto-ignition in these difficult study conditions. As a result, new testing methodologies and dedicated analyses have been developed[1]: these have cast new light on the physical phenomena triggering auto-ignition (local thermal conditions, differential evaporation of fuel components, etc.).

Expertise acquired in the field of combustion diagnosis (see figure) and analysis has led to a clearer understanding of the phenomena involved, something that is essential if we are to develop efficient new combustion systems.

Research is continuing, with examination of the role played by fuel/lubricant interactions. Another objective is to more accurately characterize auto-ignition modes[2].



Endoscopic visualization of pre-ignition in a piston engine.

(1) J.M. Zaccardi, L. Duval, A. Pagot, SAE Int. J. Engines, 2009, 2(1), 1587-1600. DOI: 10.4271/2009-01-1795

(2) J. Rudloff, J.M. Zaccardi, S. Richard, J. Anderlohr, Proc. Combust. Inst., 2013, 34(2), 2959-2967. DOI: 10.1016/j.proci.2012.05.005

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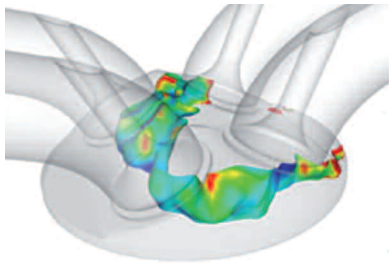
Diluting to consume less

Combustion in a reactive mixture diluted by burned gases, at high torque, is presently considered a key element for the development of modern engines. In the case of spark-ignition engines, dilution can in particular help increase efficiency. However, high dilution rates can lead to an increase of cyclic variability, which it is necessary to control.

In order to optimize the usage of high dilution rates, a number of scientific hurdles need to be overcome with respect to the impact of the dilutants on the chemical kinetics of combustion, the turbulent combustion characteristics, ignition and flame propagation, amongst others.

Understanding and mastering physical mechanisms have become major axes for IFPEN as part of its scientific involvment for the development of the engines of the future. To achieve these goals, IFPEN relies in particular on validated simulation tools. In this context, IFPEN has played a key role in the development of 3D CFD tools based on the *large-eddy simulation (LES)* approach, an area in which it has become a world leader. These tools are well suited to the simulation of reactive flows in internal combustion engines. Indeed, LES has been shown to be essential when studying abnormal combustion and cyclic variability resulting in particular from high dilution rates.

The performed studies have on one hand helped identifying the main phenomena responsible for these variations[1], and on the other hand made it possible to integrate the results of complex 3D simulations into 0D system simulation tools. Today, the latter are an important vector for promoting the use of LES applied to internal combustion engines.



LES of a pre-mixed flame in a homogeneous-charge spark-ignition engine (Lecocq et al.[2]).

(1) B. Énaux, V. Granet, O. Vermorel, ***C. Lacour, C. Pera, C. Angelberger,*** *T. Poinsot,* LES study of cycle-to-cycle variations in a spark ignition engine, *Proc. Combust. Inst., 2011, 33(2), 3115-3122. DOI: 10.1016/j.proci.2010.07.038*

(2) G. Lecocq, S. Richard, J.-B. Michel, *L. Vervisch,* A new LES model coupling flame surface density and tabulated kinetics approaches to investigate knock and pre-ignition in piston engines, *Proc. Combust. Inst., 2011, 33(2), 3105-3114. DOI: 10.1016/j.proci.2010.07.022*

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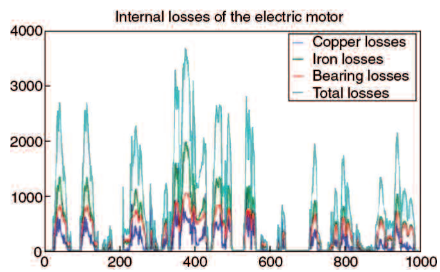
Electric vehicle motors: things are heating up!

Vehicle traction requires a significant amount of power, but for a limited period of time. Consequently, sizing an electric machine for this type of use is very different from sizing an industrial machine. For each vehicle application, it is necessary to optimize the specific power/efficiency compromise without forgetting cost constraints, which is a constant factor in the motor vehicle sector.

Optimized sizing of an electric machine therefore requires the use of multi-physical models (electromagnetic modeling, including the magnetic saturation of materials, coupled with thermal modeling) that are rapid enough to be able to be used in system simulation and coupled with an optimization tool. The approach adopted by IFPEN is based on an electromagnetic model using reluctance networks to describe the circulation of magnetic flux. For each machine technology, the reluctance network pattern is identified from the field lines and induction levels calculated by finite elements. In addition, magnetic saturation is taken into account by non-linear reluctance. In the optimization phases, this network is recalculated via a simplified extrapolation model developed by IFPEN. This magnetic model is then coupled to an equivalent first-generation electric circuit-type thermal model integrating all the thermal transfers within the machine.

The global modeling approach applied in this way for electric traction machines enables optimum sizing for each application. It thus provides the appropriate level of modeling for simulation and overall optimization of the vehicle.

Future studies will focus on improving the thermal model for the electric machine.



Calculation of losses for a real machine on the basis of vehicle use (Artemis Urban cycle).

S. Küttler, *K. El-Kadri Benkara, G. Friedrich,* ***F. Vangraefschèpe, A. Abdelli,*** Analytical model taking into account the cross saturation for the optimal sizing of IPMSM, *Conf. ICEM 2012 Marseille, 2-5 September 2012.*

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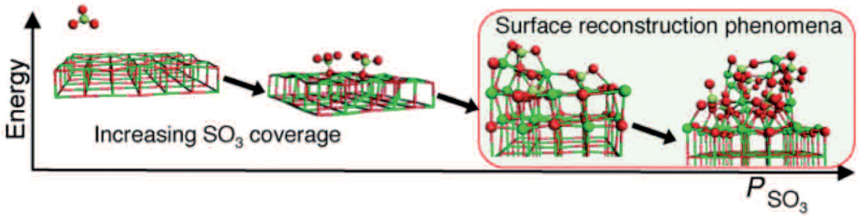
Catalytic converters: a poisoning model



Impact of reconstruction induced by SO_3 on the thermodynamic properties of the trapping material, results obtained by ab initio calculations[2].

Motor vehicle pollution control systems (catalytic converters) are subject to tightening requirements in terms of their durability. Their activity needs to be guaranteed, as verified by an onboard diagnosis tool (OBD) or in-service control (ISC). Poisoning of the catalyst with sulfur, from either the fuels or the lubricant is particularly problematic for the operation of after-treatment systems, including NO_x traps. Understanding and controlling the processes leading to poisoning are therefore crucially important for the motor vehicle industry.

As part of a joint project with Renault and the CNRS[1], IFPEN has conducted experimental studies on the sulfation and regeneration of a commercial NO_x trap, combining infrared spectrometry, X-ray diffraction and electron microscopy. Two types of sulfur species have been identified: covalent (surface) and ionic (bulk). In addition, the study demonstrated that the aging mode has a significant impact on the structural condition of the storage material and hence its poisoning mechanism: oven aging differs from that encountered onboard the vehicle.

These differences were interpreted and explained as part of a multi-scale approach based on molecular modeling. This approach makes it possible to closely examine the bond formation and rupture processes on an atomic scale and to generate thermokinetic data that can then be used by an industrial model[2]. A poisoning model based on quantum calculations has therefore been developed and is able to explain both the displacement of the sulfates formed from the bulk towards the surface of the storage material, and the reconstruction of the latter, observed experimentally. This model is now integrated into the system simulation tools developed by IFPEN for the design and control of after-treatment components. ■

*(1) **S. Benramdhane, C.-N. Millet, E. Jeudy, J. Lavy,** V. Blasin Aubé, M. Daturi, Catalysis Today, 2011, 176(1), 56-62. DOI: 10.1016/j.cattod.2011.03.049*

*(2) **N. Rankovic, C. Chizallet, A. Nicolle,** P. Da Costa, Chemistry – A European Journal, 2012, 18(34), 10511-10514. DOI: 10.1002/chem.201103950*

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Towards inoxidizable fuels

The parallel increase in the technical complexity of injection systems and fuel formulations is made necessary by ever more stringent environmental requirements.

The growing use of alternative fuels (biodiesel) and advanced conversion treatment processes for the production of diesels and jet fuels leads to a reduction in the oxidation stability of the products. At the same time, an increase in injection pressure and the use of multi-injection have significantly increased sensitivity to clogging phenomena, particularly for diesel engines. To this can be added the increasingly widespread use of hybridization, which can prolong fuel storage times in the tank.

To guarantee resistance over time and prevent failures, it is therefore necessary to gain an accurate understanding of the phenomena involved in the formation of these deposits — with potentially critical consequences —, particularly for aircraft turbines.

To achieve this, the strategy adopted is based on:
- an in-depth knowledge of the fuels themselves, both to control their formulation and perform accurate characterization;
- as well as an original approach to characterization of the varnishes and deposits formed.

Studies are being carried out on different scales in order to mimic these deposits, starting with the simplest system (oxidation of the fuel in a regulated chamber) and proceeding to the most complex one (engine), via the injection system. This sequential approach makes it possible to highlight the key parameters at each stage (chemistry, thermodynamic conditions, catalytic effects, etc.) and hence to accurately identify the processes involved. The research should ultimately lead to modeling of the phenomena and help us define solutions to solve the problem. ■

Fuel changes during oxidation phases.

***L. Starck,** M. Sicard, F. Ser, **N. Jeuland,** Potential of alternative fuels for aircraft: focus on thermal and oxidation stability, IASH 2009, Prague, Czech Republic, 18-22 October 2009.*

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ENC: strenght in numbers

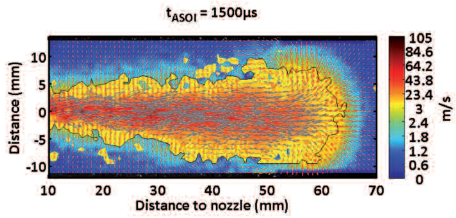
Diesel combustion systems are evolving in line with environmental and economic requirements. Two research priorities are emerging: firstly, improvement of "conventional" combustion and, secondly, the development of new combustion modes offering a better NO_x/particle compromise. Irrespective of the process envisaged, this requires an in-depth understanding of all the physicochemical processes involved in combustion, from mixture formation to soot oxidation.

The number of parameters involved, their extremely broad variation ranges and the strong interactions between them and the engine environment, are such that it is very difficult for a single research institution to tackle the problem in its entirety.

This is the reason why Sandia National Labs (United States) created the ECN (Engine Combustion Network) in 2008, in order to pool the international research in the field of diesel spray, whether experimental or focusing on modeling. IFPEN was the first research center to join this network, in 2009, conducting the network's first study jointly with Sandia, and co-organizing the first two ECN workshops.

The sharing of the experimental results obtained by the various institutes via this network makes it possible to take advantage of the complementary expertise available, define new standards for measurement methods and reinforce interactions between experiments and simulation. It also enables IFPEN to more effectively control its testing facilities. In 2012, IFPEN was thus able to measure the aerodynamic field around and inside the spray.

Although just starting, the collaboration within the ECN is already growing fast, as confirmed by the doubling in the number of participants attending the second workshop in September 2012. The network is therefore opening its doors to new institutions and will tackle new themes, such as new boundary conditions, more complex diagnostics and increasingly advanced comparison between 3D models and experiments.



Example of velocity field around (red arrows) and inside (grey arrows) the diesel spray. The color scale represents the velocity norm.

M. Bardi, R. Payri, ***L.-M. Malbec, G. Bruneaux,*** *L.M. Pickett, J. Manin, T. Bazyn, C. Genzale,* Engine Combustion Network (ECN): Comparison of Spray Development, Vaporization and Combustion in Different Combustion Vessels, *Atomization and Sprays, pending publication.*

M. Meijer, B. Somers, J. Johnson, J. Naber, S.-Y. Lee, ***L.-M. Malbec, G. Bruneaux,*** *L.M. Pickett, M. Bardi, R. Payri, T. Bazyn,* Engine Combustion Network (ECN): Characterization and Comparison of Boundary Conditions for Different Combustion Vessels, *Atomization and Sprays, pending publication.*

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HDR

• ***António Pires da Cruz,*** *HDR at the Institut National Polytechnique (INP) in Toulouse: "Modeling chemical kinetics and turbulence interactions for internal combustion engine reactive flow simulations" (15 November 2012).*

• ***Carlos Nieto,*** *HDR at Paris-Sud University: "Application of molecular simulation to thermo-physical property calculations in the field of fuels and* CO_2 *capture/storage" (27 November 2012).*

• ***Véronique Lachet,*** *HDR at Blaise Pascal – Clermont-Ferrand II University: "Molecular simulation: a tool serving industry. Application to carbon dioxide capture and storage operations" (19 December 2012).*

• ***Marc Fleury,*** *HDR at Paris Diderot-Paris 7 University: "Characterization of porous media via electric properties and magnetic resonance" (9 January 2013).*

Awards

• **Kirsten Leistner,** *a PhD student, was awarded the Gérard De Soete 2012 prize for her thesis entitled "Experimental study and modeling of catalytic oxidation of diesel soot" (29 November 2012).*

• **François Roure,** *Expert Director, was awarded the André Dumont prize by Geologica Belgica following the association's AGM (7 March 2013).*

Scientific visitors

• ***Paulo de Souza Mendes,*** *a Professor at Pontifícia Universida de Catolica (Rio de Janeiro, Brazil), was hosted by IFPEN from 3 September 2012 to 28 February 2013, within the Applied Mechanics Division.*

• ***Camilla Gambini Pereira,*** *a Professor in the Chemical Engineering Department at Rio Grande do Norte Federal University (Brazil), has been hosted within the Applied Chemistry and Physical Chemistry Division since 4 March.*

• ***Faiçal Larachi,*** *a Professor in the Faculty of Science and Chemical Engineering at Laval University (Canada) has been hosted within the Process Design and Modeling Division since 1 March.*

Upcoming scientific events

• *PetroPhase 2013* ***– Petroleum Phase Behavior and Fouling –*** *10-13 june 2013, IFPEN Rueil-Malmaison*

• *IFP Energies nouvelles' "Rencontres scientifiques" event* ***– Viscoplastic Fluids: From Theory to Application –*** *18-21 november 2013, IFPEN Rueil-Malmaison*

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