



# Science@ifpen

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*The transportation sector is evolving all the time and profound changes are yet to come. A major challenge for future mobility,*

*vehicle's electrification will be accompanied by radical technological and software advances, with the increasing development of connected and driverless vehicles, incorporating, in particular, the principles of responsible eco-driving.*

*For all that, Internal Combustion (IC) engines will continue to dominate for a few more years to come. The focus must be on reducing their consumption (i.e. decreasing CO<sub>2</sub>) and their pollutant emissions, paving the way for the transition to low-carbon mobility.*

*In addition to the development of new software solutions and services for vehicle electrification and connected mobility, researchers from the Powertrain and Vehicle Division are channeling their expertise into addressing these challenges. Their aims today: to prepare for the changes that will take place in the distant future while going on improving the short term, essential for addressing the needs of industry and society, working in partnership with internationally-recognized laboratories.*

*I hope you enjoy reading this issue.*

Stéphane Henriot,  
Director of the Powertrain and Vehicle Division

## Observation of soot in a diesel flame

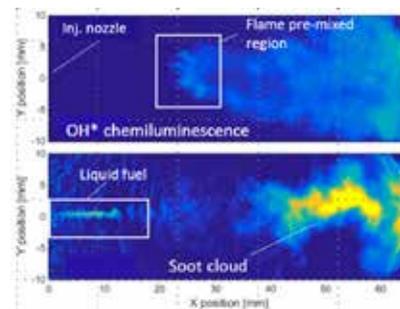
The reduction in IC engine particle emissions requires a detailed knowledge of the physicochemical processes at work during combustion. While fuels have long since been considered as a constant for each engine type, the gradual introduction of biofuels and research conducted in the field of innovative combustion modes have made it necessary to take greater account of the impact of fuel variability on pollutant formation.

The task is painstaking since fuels are made up of thousands of hydrocarbon compounds and accurately reproducing their behavior is beyond the scope of chemical modeling. Moreover, standard characterization tests (for example, cetane number) are not sufficiently descriptive.

In order to understand the relationship between fuel properties and soot formation in a diesel-type combustion scenario, an innovative characterization model was set up by IFPEN's researchers. The model is hinged around a high-pressure and high-temperature chamber and employs advanced optical measurement techniques with a view to obtaining a simultaneous picture of (figure):

- reaction zones, by chemiluminescence<sup>a</sup>;
- the quantitative distribution of soot in the flame, via 2D extinction<sup>b</sup> measurement.

The use of these techniques demonstrated that fuel composition acted independently on several aspects of combustion, including



*Simultaneous images of the reaction zone (top) and soot distribution (bottom).*

the two principal factors influencing soot formation in the flame: equivalence ratio in the pre-mix zone and local chemistry.

The impact of different families of hydrocarbons<sup>c</sup> was characterized in representative engine operating conditions<sup>(1)</sup> and this new method could also be used either to evaluate new fuels or to validate surrogate fuels used in computational simulation tools. ■

a - Measurement of light emitted by a chemical reaction.  
b - Light absorption measurement.  
c - Such as long-chain aliphatic alkanes (n-dodecane) or aromatics (n-propylbenzene).

(1) M. Bardi, G. Bruneaux, O. Colin, SAE Technical Paper 2017-01-0721, 2017.  
DOI: 10.4271/2017-01-0721

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IFP Energies nouvelles (IFPEN) is a major research and training player in the fields of energy, transport and the environment. From research to industry, technological innovation is central to all its activities.



# LES moves to rapid transients for cleaner powertrains

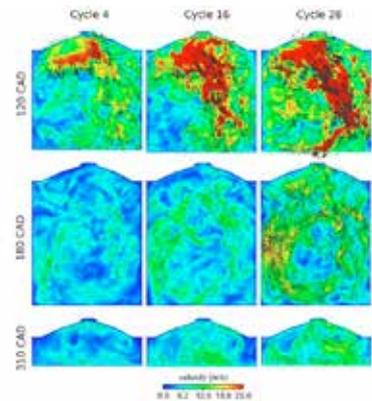
Gasoline direct injection engines emit soot particles during rapid transients. This still poorly understood phenomenon is taken into account during new WLTCs<sup>a</sup>, aimed at more accurately reproducing real vehicle use.

High-resolution, digital flow simulations in the combustion chamber, capable, in particular, of resolving cycle-to-cycle variations, can be used to gain a better understanding of the mechanisms behind this soot formation. However, these simulations, based on LES<sup>b</sup>, are mastered on stabilized operating points<sup>(1)</sup>, where they give relevant results, but they have never been carried out for transients.

Research conducted by IFPEN<sup>(2-3)</sup> in the ANR Astride<sup>c</sup> project demonstrated the relevance of LES for tackling this problem, via the first ever calculations involving 1D-3D code coupling. In particular, these simulations reproduced the impact of engine transients, i.e. engine speed variations (for example, acceleration between 1,000 rpm and 1,800 rpm in the figure), on the acoustics in the intake line, and

thus on filling and aerodynamics in the combustion chamber.

Further work is now required to fine-tune the results, separating the average and fluctuating components of velocity ranges. To do this, research is focusing on two areas: obtaining a usable average based on several transients, and the implementation of specific after-treatment analyses, such as EMD<sup>d</sup> <sup>(4)</sup>.



LES resolution of instantaneous velocity ranges for three crankshaft angles, and for three transient cycles: cycle 4 (1,000 rpm), cycle 16 (1,400 rpm) and cycle 28 (1,800 rpm).

(1) A. Robert, S. Richard, O. Colin, L. Martinez, L. de Francqueville and al, *Proc. Combust. Inst.* 35(3), 2015.

(2) B. Roux, *IFPEN, PhD thesis* 2015.

(3) A. Poubeau, S. Jay, A. Robert, E. Nicoud and al., *SAE Technical Paper* 2017. DOI: 10.4271/2017-24-0028

(4) M. Sadeghi, K. Abed-Meraim, F. Foucher, C. Mounaïm-Rousselle, *iTi Conference on Turbulence, Bertinoro, Italy, Sept. 2014.*

- a - Worldwide harmonized Light vehicles Test Cycles.
- b - Large-Eddy Simulation.
- c - Aerodynamics and Sprays during Transients of Gasoline Direct Injection Engines.
- d - Empirical Mode Decomposition.

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## Where aviation fuels are concerned... compromise is the name of the game

In the aviation sector, fuels derived from hydrotreated vegetable oils (HEFA<sup>a</sup>) are seen as an alternative to petroleum based Jet A-1<sup>b</sup> to reduce the environmental footprint of air transport. However, the use of these primarily paraffinic alternative fuels may generate problems related to circuit impermeability. To avoid this issue, a minimum aromatic content is needed, since aromatics are absorbed by polymer seals, ensuring their expansion. However, the quantity of these compounds needs to remain limited since they cause deposits and pollutant formation.

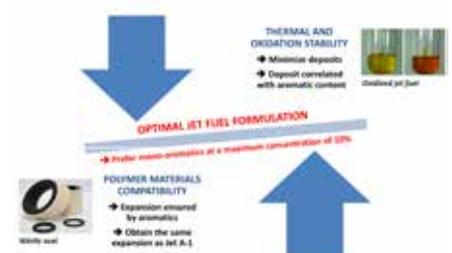
The optimization of the formulation of synthetic aviation fuels was the focus of the CAER<sup>c</sup> project. A dedicated experimental research program was conducted on materials compatibility, thermal stability and oxidation resistance tests<sup>(1)</sup>.

Using cutting-edge techniques, IFPEN's teams thus investigated the various mechanisms involved in thermal and oxidation stability, also combining measurements on real fuels and model fluids. The latter were produced from

a HEFA-type paraffin base, to which aromatics (xylene or tetraline) were added at various concentrations.

Finally the need to have aromatics present to swell the seals was confirmed, with an effect equivalent to that produced by Jet A-1 fuel for the addition of 10% v/v of either one of the compounds tested. Optimal compositions were also identified for oxidation and thermal stability. Ultimately, the results suggest that a formulation favoring monocyclic aromatics such as 10% xylene v/v represents the best compromise for all of the properties studied<sup>(2)</sup>.

The work is continuing in order to expand the database in terms of chemical compounds, and with a view to develop a predictive modeling approach which determines properties vs composition relationships. ■



Jet fuel formulation optimization.

- a - Hydroprocessed Esters and Fatty Acids.
- b - Fuel used in the aviation sector.
- c - Alternative fuels for the aviation sector, coordinated by IFPEN.

(1) A. Ben Amara, M.-H. Klopffer, B. Veyrat, L. Starck, *International Congress and Expo on Biofuels & Bioenergy, August 29-31, 2016 Sao Paulo, Brazil.*

(2) A. Ben Amara, M.-H. Klopffer, M. Alves Fortunato, L. Starck, *Optimal jet fuel composition with stability and improved oxidation. Patent WO 2017/050687 A1.*

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# Life and death of soot: a model to control the phenomenon

Vehicle approval standards require increasingly high levels of engine performance (low fuel consumption and low emissions) over a broad working range. It is for this reason that new engine architectures incorporate technologies such as direct injection and burned gas recycling systems, two levers for combustion optimization. In this context, engine control strategies are becoming extremely sophisticated, hence increasing recourse to system simulation.

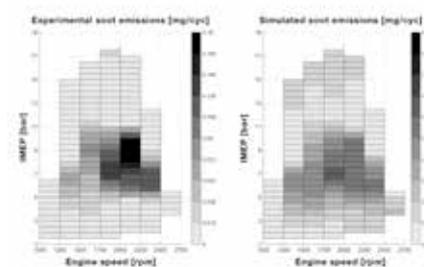
However, the complexity of the mechanisms involved in the formation of pollutants in the combustion chamber, particularly soot, makes their detailed incorporation in traditional system simulation approaches difficult. To overcome this difficulty, IFPEN has developed phenomenological models, i.e. based on the physics of phenomena but using more global descriptors.

Significant correlations exist between soot emissions and the thermochemical conditions of the fuel-air mixture at known and specific locations within

the diesel fuel jet<sup>(1)</sup>: particularly at the lift-off length (region where soot forms) and within the diffusion flame (location of soot oxidation). These factors are themselves directly related to the engine control parameters.

This knowledge has formed the basis for the development of a model capable of describing such conditions throughout the engine cycle<sup>(2)</sup> and, from this, deducing a quantitative prediction of soot formation (figure). The model obtained, which also makes it possible to predict the impact of adjustment variations with respect to a given operating point (injection strategy, dilution ratio, turbocharging rate), was incorporated in the IFP-Engine library for the Simcenter Amesim<sup>TM</sup> <sup>a</sup> software marketed by Siemens.

The challenge now is to cover a broader range of engine operating conditions, and, in order to do so, to establish the applicability of the correlations employed. ■



Comparison of measured and calculated soot quantities for a running engine<sup>b</sup>.

a - Multi-physical simulation tool.  
b - IMEP: Indicated Mean Effective Pressure.

[1] L. Pickett, D. Siebers, *Combustion and Flame*, 138: p. 114–135, 2004

[2] A. Dulbecco, G. Font, *SAE Technical Paper 2017-24-0022*.  
DOI: 10.4271/2017-24-0022, 2017

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In order to reduce fuel consumption in gasoline engines, manufacturers are focusing their efforts on turbocharging and downsizing. However, this option leads to an increase in the knock phenomenon (destructive engine self-ignition). This can be avoided by significantly increasing the dilution ratio using re-circulated burned gases, but such an approach is to the detriment of flame stability during spark ignition, and hence to the detriment of engine stability.

In this context, manufacturers have turned to CFD<sup>a</sup> and, in particular, LES<sup>b</sup> in order to understand the causes of – and thereby address – cycle to cycle fluctuations which reduce engine stability. However, existing combustion models capable of describing spark ignition, do not take sufficient account of these fluctuations.

To develop such a model<sup>(1)</sup>, IFPEN took part in the Famac<sup>c</sup> project, providing an electric circuit model for a standard vehicle coil, capable of accurately reproducing the energy transferred by the spark plug.

Since energy is deposited along the electric arc, this first model was then supplemented by a Lagrangian arc model, which reproduces the shape and evolution of the real arc (figure 1).

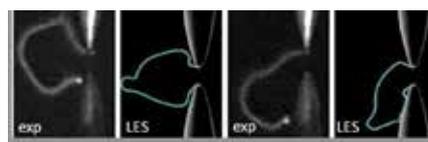


Fig. 1 - Experience vs LES comparison for the two electric arc images.

This approach made it possible to correctly simulate the critical ignition energy at rest, without turbulence (figure 2). The first calculations for “standard engine conditions” (with turbulence) also demonstrated good consistency with experience.

These first models representing complex ignitions in turbulent conditions will be evaluated for concrete cases and be used to propose ignition strategies designed to reduce knocking. Ultimately, they will also be used to help design the new, more robust ignition systems

## Ignition simulation

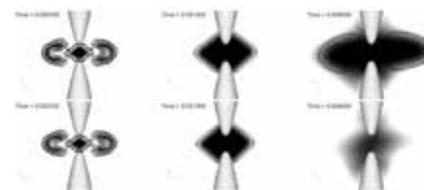


Fig. 2 - Propane/air ignition at rest. 107 mJ (top) and 78 mJ (bottom) of energy leading to ignition success and failure respectively.

that will form the basis of more fuel-efficient, cleaner engines. ■

a - Computational Fluid Dynamics.  
b - Large-Eddy Simulation.  
c - Ignition fundamentals for the spark ignition engine.

[1] O. Colin and al., “DNS and LES of spark ignition with an automotive coil”, submitted for the *Symposium on Combustion 2018*.

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# Pollutant emissions: better knowing them to fight them better

Vehicle approval certifies that the emissions of said vehicle meet the specifications imposed by existing standards. Although current regulations only concern a limited number of chemical species, the impact of the latter on human health and the environment is leading to a tightening up of legislation, with a reduction in emission thresholds and the inclusion of new pollutants. Consequently, there is a need for a more in-depth understanding of the various types of chemical species emitted and their concentrations, depending on vehicle operating modes.

To address this need, IFPEN coordinated two projects that shed light on emissions – regulated or not – from vehicles representative of the French market.

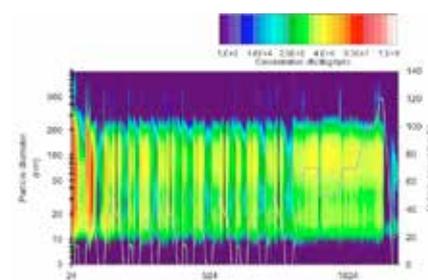
The Cappnor project highlighted:

- high levels of ultra-fine particle emissions from a gasoline direct injection powertrain (figure),
- the very high efficiency of Diesel particle filters, thanks to which the exhaust emission concentrations are indistinguishable from urban atmospheric levels<sup>(1)</sup>.

The Cappnor 2 project demonstrated that the efficiency of the two major technologies aimed at reducing nitrogen oxide emissions (NOx)<sup>a</sup> of Diesel engines was heavily dependent on the way they were implemented by manufacturers within the various engine operating ranges<sup>(2)</sup>.

Vehicle approval procedures evolved in 2017 to ensure low emission levels over a broader range of use of an internal combustion engine. The results of these two projects provide legislators with a basis for defining improved emission reduction measures. They also indicate the development priorities that IFPEN should be focusing on in terms of designing new pollution control systems.

In parallel, the continuous improvement process is being pursued with the Rhapsodie project, focusing on the various forms of polycyclic aromatic hydrocarbons present in particles and in the gas phase. ■



Particle concentrations (color) emitted by a gasoline direct injection vehicle: evolution over time depending on their diameter when speed varies (gray curve)<sup>b</sup>.

- a - Catalytic reduction using urea (SCR Selective Catalytic Reduction) and NOx trap (LNT: Lean NOx Trap).  
b - When the speed (gray curve) and the temperature entering the catalytic converter (red curve) are varied.

[1] S. Zinola, S. Raux, M. Leblanc, SAE Technical Paper 2016-01-2283, 2016.  
DOI: 10.4271/2016-01-2283

[2] M. Leblanc, L. Noël, B. R'Mili, A. Boréave, B. D'Anna, S. Raux, Journal of Earth Sciences and Geotechnical Engineering, vol.6, no. 4, 2016, 29-50

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## News

• In 2017, IFPEN filed 187 patents, including 79 related to New Energy Technologies (NETs), breaking its previous record from 2016.

• The 2018 IFPEN Panorama conference on the "Energy transition: the role of territories and technological challenges" took place on 8 February. Associated publications and full conference footage are available on the [www.panorama-ifpen.fr](http://www.panorama-ifpen.fr) website.

## Award

• The French Rock Mechanics Committee awarded the 2017 Pierre Londe thesis prize to Bertrand Paul, a PhD researcher at IFPEN, for his thesis in the field of geomechanics, carried out in collaboration with EDF R&D and the University of Lorraine.

## Upcoming scientific events

• The IFP Energies nouvelles "Rencontres scientifiques" event **Solid Liquid Interfaces, Molecular Aspects for Industrial Applications [SLIMIAI]**, 27 to 29 March 2018, IFPEN Rueil-Malmaison - [www.rs-slimaia.com](http://www.rs-slimaia.com)

• Workshop **Commodities and Energy Market Organization in the Energy Transition Context [EM 2018]**, 18 and 19 June 2018, IFPEN Rueil-Malmaison - [www.ws-em2018.com/](http://www.ws-em2018.com/)

## Publications

• IFPEN's Scientific Division has published its 2017 brochure "IFP Energies nouvelles, fundamental research serving innovation". It is available in pdf format on the IFPEN website: [www.ifpen.fr](http://www.ifpen.fr).

• IFPEN contribution to an ebook on *The Conversation* – free online media – for a better understanding of the issues and challenges surrounding the energy transition – [www.theconversation.com](http://www.theconversation.com)

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