Science@ifpen
Issue 7 - May 2011

We have been publishing the latest scientific results achieved by our researchers in this newsletter for a number of years now and this issue is no exception. However, one thing that sets it apart is its new context. IFP has changed its name and is now known as IFP Energies nouvelles (IFPEN). This name change reflects a shift in our strategy, initially oriented mainly towards oil and gas and now largely focusing on new energy technologies (hybrid and electric vehicles, biofuels, green chemistry, CO_2 capture and storage, etc.). As a result, Science@ifp has also changed its name to become Science@ifpen. However, over and above the technological breakthroughs necessary to bring about these changes, the approach proposed by IFPEN demonstrates a high level of continuity. Because the determination to generate innovations that has driven IFPEN's researchers from the very outset has led it to develop exceptional expertise, now channeled into meeting these new challenges.

This will become obvious to readers when they discover the research presented in this newsletter.

We hope that you enjoy this issue,

Sophie Jullian
Scientific Director

Engine diagnosis using laser technology

The development of increasingly efficient and ever cleaner engines requires precise measurement of gas temperatures in the combustion chamber since the temperature has a direct impact on the formation of the air-fuel mixture, self-ignition and pollutant formation.

However measurement is made difficult by the engine environment. What's more, the very marked temperature sensitivity of the phenomena studied demands a very high level of precision.

These non-intrusive optical diagnostic techniques are particularly suitable for obtaining information of this type. In particular, numerous studies have demonstrated the potential of laser induced fluorescence for temperature measurement. However, its application in a diesel jet, characterized by marked temperature gradients, is still a major challenge.

It is against this background that IFPEN has developed this technique in a high-pressure cell enabling the thermo-dynamic conditions of the diesel engine to be reproduced. An original methodology has been implemented to simultaneously optimize the experimental set-up, image processing and measurement error, as well as quantify the latter.

The results obtained have proved to be highly satisfactory. Temperatures of up to 700K have been measured, with a precision of ±20K and a systematic error of less than ±30K.

A promising first step has therefore been taken and it will be necessary to continue developing the technique to include simultaneous temperature and fuel and oxygen concentration measurements, in order to gain an even more precise understanding of the physical phenomena at play.

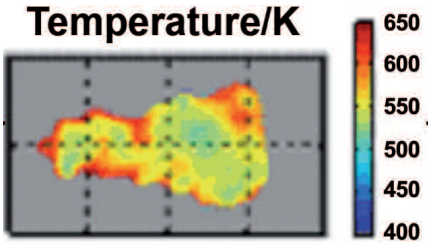

Image of the temperature in a non-reactive diesel jet obtained by laser induced fluorescence.

R.Devillers, G.Bruneaux, *C.Schulz, Appl. Phys. 96 (2009) 735-739*
G.Tea, G.Bruneaux, J.Kashdan, *C.Schulz, Proc. Combust. Inst. 30 (accepted for publication - 2010)*

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Atomizing aluminosilicates!

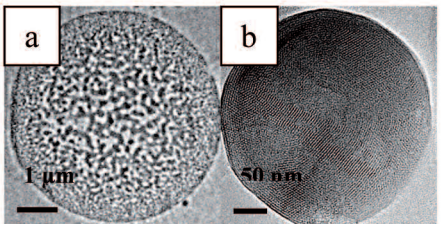
In addition to their conceptual value, solids with a uniform and organized ("mesostructured" materials) and/or hierarchized (variable porosity range from micro- to macroporosity) porosity offer promising prospects for the catalyst industry, which is keen to develop ever more efficient and environmentally-friendly products.

IFPEN and the *Laboratoire de Chimie de la Matière Condensée de Paris* (LCMCP – Paris Laboratory for Condensed Matter Chemistry) have been working together to address this challenge since 2002. Adopting an original approach, they have focused on a specific technology: atomization (or aerosol).

In this way, they have been able to use a continuously operating tool to obtain, in a single synthesis step, mesostructured aluminosilicates with a high aluminum content, composite solids composed of zeolite nanocrystals trapped in a mesostructured matrix and micro-, meso- and macroporous aluminosilicates, structured or otherwise.

This technology offers two advantages: first of all, it can be used to create a multitude of solids. Secondly, it appears to be compatible with the challenges of industrial-scale production. In addition, the unusual acidity properties of some of the materials obtained, totally different from those of acidic solids used industrially for catalysis, open up potential new research and development avenues in the fields of innovative materials and catalysis.

This is a particularly promising avenue given the tense energy context in which technological innovation will play a predominant role in meeting our needs.



a) Particle with a hierarchized porosity, mesoporous at the edges, macroporous in the center.

b) Mesostructured particle with cylindrical pores distributed periodically through the matrix.

A. Chaumonnot, *F. Tihay, A. Coupé, S. Péga, C. Boissière, D. Grosso, C. Sanchez, Oil and Gas Science and Technology-Rev.IFPEN, 64, 6 (2009) 681. DOI: 10.2516/ogst/2009029*

S. Péga, C. Boissière, D. Groso, T. Azaïs, ***A. Chaumonnot,*** *C. Sanchez, Angew. Chem. Int. Ed. 48 (2009) 2784. DOI: 10.1002/anie.200805217*

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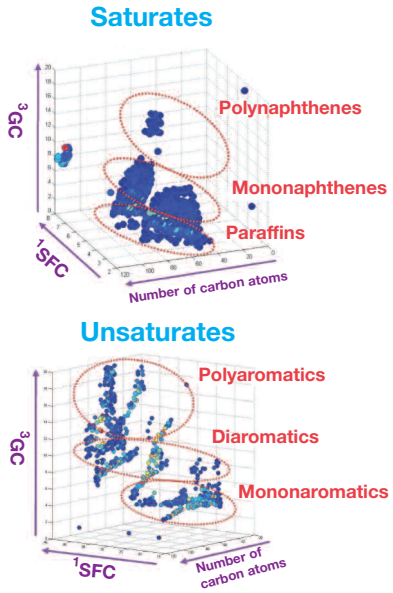
Vacuum distillates seen under a totally new light



3D chromatograms produced by analysis of a vacuum distillate by SFC / GC2D-HT coupling.

In order to meet the increasing energy demand in a context of expected cap on fossil fuel availability, it is essential to convert as much petroleum as possible into fuels. Vacuum distillates conversion processes play a major role in achieving this goal but require detailed analytical data for their optimization via kinetic modeling.

Although detailed molecular information is available for lighter cuts such as gasoline or diesel cuts, few structural information is available for vacuum distillates, due mainly to the number of components they contain (over a million).

Recently, the use of high-temperature two-dimensional gas chromatography (HT-2D-GC) led to strong advances in the analysis of hydrocarbons in vacuum distillates. However, two separation dimensions did not provide sufficient analytical details.

Improvement of the separation power of this technique was performed at IFPEN by adding an online SFC (Supercritical Fluid Chromatography) separation dimension, which allows the pre-fractionation of compounds according to their chemical family. Its hyphenation to HT-2D-GC resulted in unprecedented analytical details on vacuum distillates and a 3D representation of the hydrocarbons distribution was proposed.

This kind of analytical tools proves to be of major importance for the study of conversion processes but may also be extended to the analysis of other complex matrices, such as those produced in biomass transformation processes.

T. Dutriez, M. Courtiade, *D. Thiébaut,* ***H. Dulot, F. Bertoncini, J. Vial,*** *et al., HT-2D-GC of hydrocarbons up to nC (60) for analysis of vacuum gas oils, J. Chrom. A, 1216, (2009) p.2905-2912, DOI: 10.1016/j.chroma. 2008.11.065*

T. Dutriez, M. Courtiade, *D. Thiébaut,* ***H. Dulot, F. Bertoncini,*** *et al., Extended characterization of a vacuum gas oil by offline LC-HT-2D-GC, J. Sep. Sci., 33 (2010) p.1787-1796, DOI: 10.1002/jssc.201000102*

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Biofuels turn to fungus

The production of 2nd-generation bioethanol requires the action of enzymes, generally derived from the filamentous fungus *Trichoderma reesei.* These enzymes are obtained by cultivating the fungus in a fermenter. However, the cost of this process is still too high. One of the avenues being explored to bring down the cost is improving the performance of *T. reesei* strains by genetic engineering.

The challenge for molecular genetic engineers is to identify which of the several thousand genes need to be modified to improve the strain. To do this, they use genomics and systems biology techniques, enabling collection of all the cellular information (DNA sequence, expression of genes in a given culture condition, etc.). In this way, they aim to create a predictive model of micro-organism behavior.

Working closely with ENS Paris and several laboratories in Europe and the USA, IFPEN researchers have deciphered the genome of a complete lineage of *T. reesei* strains. For the first time, they have obtained an exhaustive list of the mutations that affect these strains. This work is currently being supple-mented by genetic expression studies (transcriptome) on *T. reesei*. This information will form the basis for an operational model helping to guide genetic engineering choices in order to obtain more efficient strains.

These advances will thus help bring down the cost of producing 2nd-generation biofuel.

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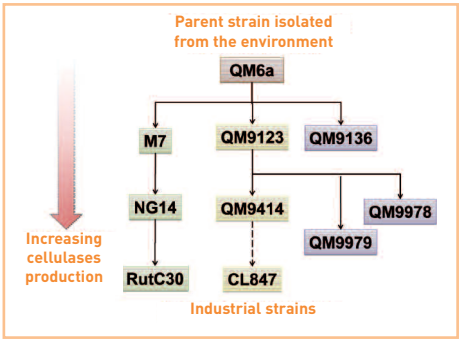

Example of T. reesei *strain lines. Comparative study of their genome leads to identification of the key genes involved in cellulase production.*

S. Le Crom, W. Schackwitz, L. Pennacchio, JK. Magnusone, DE. Culley, JR. Collett, J. Martin, IS. Druzhinina, ***H. Mathis, F. Monot,*** *B. Seiboth, B. Cherry, M. Rey, R. Berka, CP. Kubicek, SE. Baker, and* ***A. Margeot,*** *Proc. Nat. Sci. USA, Volume 106, n°38, pp 16151–16156, DOI: 0.1073/pnas.0905848106*

CO_2 on the move

It is essential to monitor the evolution of CO_2 injected into a geological reservoir to ensure that the storage site remains intact over time and to fine-tune simulation models.

Among the various geophysical methods examined (seismic data, gravimetry, electromagnetism), repetitive seismic data are emerging today as the most effective method of meeting these two objectives. However, this method is dependent on being able to interpret seismic property variations in under-ground environments due to the injection of CO_2 between two data acquisitions separated over time.

Geophysicists working within IFPEN's Geology-Geochemistry-Geophysics Division have just achieved a first, adapting interpretation techniques developed for the characterization of oil fields to the geological CO_2 storage context. As part of the European FP6 project, CO_2ReMoVe, these techniques have been applied to seismic data recorded at the Sleipner site (North Sea - Norway) during surveys conducted in 1994 and 2006 (before and after 10 years of CO_2 injection). The seismic impedance variations obtained enable monitoring of the 3D evolution of the CO_2 plume within the host saline aquifer.

The results obtained have been analyzed in order to quantify the CO_2 stored in the aquifer. Comparison of these data with reservoir simulations will help reinforce predictions relative to storage site behavior over several centuries. More broadly, the experience acquired thanks to the development and deployment of these new technologies on the first sites will enable recommendations to be drawn up relative to the management of geological CO_2 storage sites.

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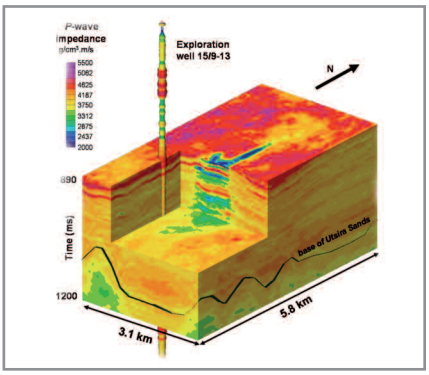


3D view of the distribution of P wave impedance obtained following seismic inversion of data acquired in 2006. CO_2 is identified by lower impedance values (blue and green colors) inside the reservoir (as per Clochard et al. *First Break 2010).*

T. Tonellot, M.-L. Bernard and ***V. Clochard****, 2010. Method of joint inversion of seismic data represented on different time scales, US Patent 2010/0004870 A1*

N. Delépine, V. Clochard, K. Labat, P. Ricarte, *2010. 2011. Post-stack stratigraphic inversion workflow applied to carbon dioxide storage: application to the saline aquifer of Sleipner field, Geophysical Prospecting, vol 59 (1), 132-144, DOI: 10.1111/j.1365-2478.2010.00905.x*

N.Dubos-Sallée and P. Rasolofosaon, 2011. Estimation of permeability anisotropy using seismic inversion for the CO_2 geological storage site of Sleipner (North Sea), Geophysics, vol 76 (3), B1–B7

Getting to grips with particles!

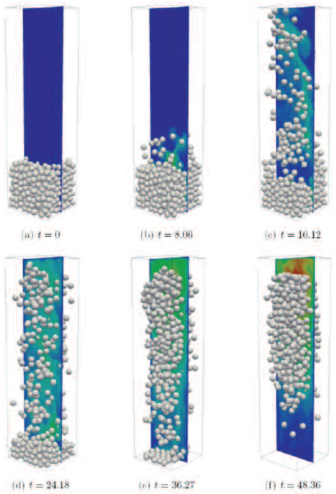
From the transport of sand in production pipelines to fluidized beds in catalytic reactors, fluid/particle flows are present in a large number of applications studied by IFPEN. Their scientific, industrial and economic importance means that understanding them is essential.

However, it is difficult to study them due to the broad range of scale in these flows, from a grain of sand to a pipeline that runs several hundred kilometers, or from the fine feedstocks to a fluidized catalytic cracker of several meters. It is therefore crucial to precisely determine the interactions between the particles and the suspending fluid on a micro scale in order to be capable of satisfactorily modeling the overall behavior on a macro scale.
For the last few years, IFPEN has been developing massively parallel 3D computational codes to directly simulate this micro scale: GRAINS3D for inter-particle collisions and PeliGRIFF for hydrodynamic coupling. Used on powerful supercomputers, these codes enable modeling of up to 100,000 particles coupled with a fluid and several million in a dry granular flow.

The development of PeliGRIFF is thus consistent with a multi-scale simulation approach. The next studies will focus on methods to integrate the results from the micro to the macro scale, in a kind of upward cascade of knowledge.

A. Wachs, A DEM-DLM/FD method for direct numerical simulation of particulate flows: Sedimentation of polygonal isometric particles in a Newtonian fluid with collisions. Computers & Fluids, 38(8), 1608–1628, 2009, DOI:10.1016/j.compfluid.2009.01.005

G. Vinay, A. Wachs, V. Hergault, DNS of particulate flows with collisions using a parallel DEM-DLM/FD method: PelIGRIFF, Vth European Conference on Computational Fluid Dynamics, ECCOMAS CFD 2010, Lisbon, Portugal



Re-suspension of 500 spherical catalysts by natural convection: temperature evolution over time.

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Nominations

• **Olivier Appert,** *Chairman and CEO of IFPEN, was elected, in early 2011, as chairman of the Conseil français de l'énergie (CFE - French Energy Council), taking over from Anne Lauvergon.*

• **Sophie Jullian,** *IFPEN's Scientific Director and Chair of the Axelera competitiveness cluster Scientific Board, was appointed Chair of Lyon's École Normale Supérieure (ENS) Scientific Board on 14 June 2010, on recommendation of Jacques Samarut as his successor. She was also appointed to the Scientific Board of INRA on 7 January 2011.*

Publications

F. Lecomte – CO_2 Capture Technologies to Reduce Greenhouse Gas Emissions – Le Captage du CO_2 – Éditions Technip – ISBN 9782710809388 (French version : Des technologies pour réduire les émissions de gaz à effet de serre)

Alain-Yves Huc – Heavy Crude Oils – From Geology to Upgrading. An Overview – Éditions Technip – ISBN 978271080890

Distinctions

• **Jérémie Dautriat** *received one of École Polytechnique's 2010 thesis prizes, for the quality of his thesis on the "Hydromechanic behavior of reservoir rocks under stress - Relationships between permeability changes and scales of damage mechanisms". Academic guidance was given by Jean Raphanel and Alexandre Dimanov from the École Polytechnique's Solid Mechanics Laboratory and this thesis was overseen by Nicolas Gland at IFPEN.*

• **Pascal Raybaud,** *an expert within the Catalysis and Separation Division, was awarded the prize from the Catalysis division of the French Chemistry Society. This prize awards significant research work which has been ongoing since 1995, making it possible to streamline and conceptualize heterogeneous and homogeneous catalysts on an atomic scale, thanks to quantum molecular modeling combined with experimental techniques.*

• **François Roure,** *an expert within the Geology-Geochemistry-Geophysics Division, was bestowed with the 2010 Wegener Award by the EAGE (European Association of Geoscientists and Engineers) in recognition of his research contribution to the understanding of thrust faults and foreland basins, as well as the effects of compressive tectonics on fluid movements.*

• **Christian Wittrisch** *received the Jury Prize on 17 January 2011 during the 10th Chéreau-Lavet prize-giving ceremony in 2010 for best engineer-inventor. He has been awarded for the invention of the Simphor, an instrumentation and measurement system for a horizontal well. He has already received two prizes for this invention which has been marketed by Vinci Technologies.*

• **IFP Energies nouvelles' Yves Chauvin thesis prize 2010:** *the prize was awarded to Ludovic Metivier, a former PhD student at IFPEN, for his thesis "A non-linear inversion method for high-resolution seismic imaging", supervised by Laurence Halpern (lecturer at Paris 13 University) and overseen by Florence Delprat-Jannaud at IFPEN.*

• **French Chemistry Society's *(Société Chimique de France)* 2010 thesis prize :** *the prize was awarded to Frédéric Biscay, a former PhD student at IFPEN, for his thesis on "Molecular modeling of high-pressure liquid-steam interfaces and prediction of interfacial tension" supervised by Patrice Malfreyt (lecturer at Blaise Pascal University in Clermont-Ferrand) and overseen by Véronique Lachet and Philippe Ungerer at IFPEN.*

Managing editor: Marco De Michelis
Editor in chief: Sophie Jullian
Editorial committee: Xavier Montagne, Emmanuelle Hutin
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ISSN No: 1957-3537

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