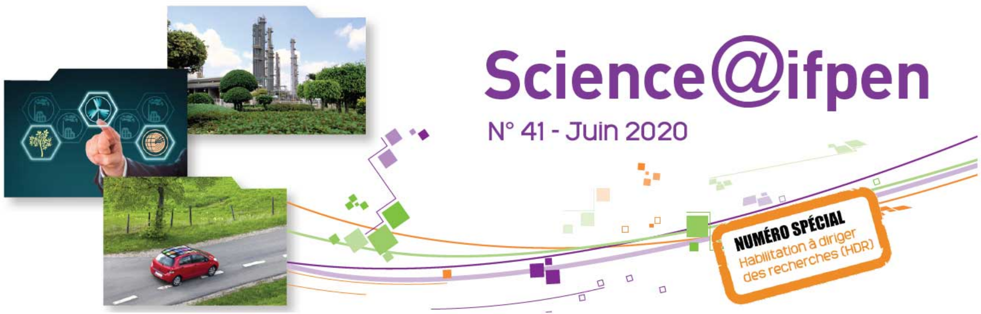


Written on 10 July 2020

15 minutes of reading

News

Fundamental Research

neering and process engineering

Research and training underpin the relevance and originality of all the innovations developed at IFPEN. Key actors in the entire process, some of our researchers are awarded a **national accreditation to supervise research (HDR), France's highest university qualification**. HDR researchers are recognized for their high level of scientific training and expertise, the originality of their scientific approach, and their capacity to develop and master a research strategy as well as supervise PhD theses. Beyond the role of indicator of scientific excellence, **the number of HDRs reflects the quality of supervision for our PhD students**, and the balanced and constructive nature of exchanges with our academic partners.

This issue highlights major results obtained by some of our researchers who have recently been awarded this title. From experimentation to modeling, covering multiple scales of time and space, the range of topics investigated and disciplines concerned is vast, reflecting the broad variety of activities at IFPEN.

A common thread runs through all this research: a coherent and long-term scientific approach that guarantees the quality and relevance of our results within the fundamental research-applied research continuum.

I hope you will enjoy reading this issue.

Olga Vizika-Kavvadias,
Scientific Director

See the PDF of the letter

LES BRÈVES

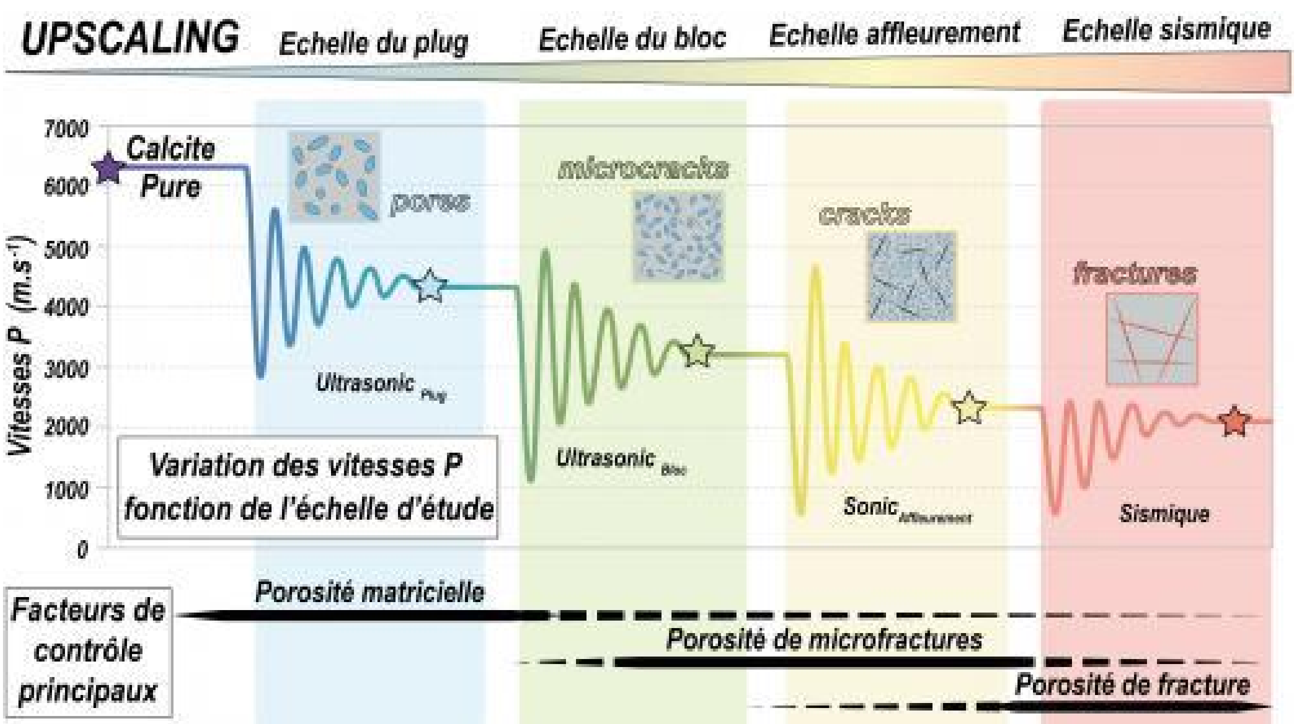
Carbonate reservoirs present significant heterogeneities (in terms of types and scales) associated with the biological origin of sediments[c], as well as the diagenetic transformations that took place when they were deposited or very soon afterwards. This facies-early diagenesis couple thus governs the initial state and evolution of future reservoirs during burial. The purpose of my HDR was to better define this initial state in order to take it into account in geological models.

This research has found direct applications at IFPEN for:

• **multidisciplinary and multiscale carbonate modeling**[d]. The idea is to identify the petrophysical and petroacoustic signatures (figure) of
the different facies and the effects of diagenetic alterations, and to demonstrate the different levels of heterogeneity (micro, meso and macroporosity) in these carbonates(1);

• **modeling of the mineralogical and petrophysical modifications** undergone by a carbonate sediment during early diagenesis, in order to develop a new module for DionisosFlow[e] 3D stratigraphic modeling software.

For the latter, the work conducted for the HDR led to the **development of phenomenological laws** incorporating several parameters, such as initial minerology, residence time in each hydrological zone and process kinetics.



Principal P-wave velocity control factors for various study scales (from plug to seismic)(1).

The carbonate sedimentary systems studied constitute highly detailed records of environmental changes (climate, sea level, population ecology, etc.), the analysis of which provides keys for understanding and modeling current challenges(2).

a - Descriptive notion of a sedimentary rock based on its appearance and composition
b - Early diagenesis, for which the chemistry of interstitial fluids is directly controlled by the surface environment
c - Which defines the different types of carbonate facies
d - Within the context of the research conducted by C. Bailly (ENS 2019) or the Aquarius consortium
e - Integrated numerical geological model including sedimentary processes

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(1) C. Bailly, M. Adelinet, Y. Hamon, J. Fortin, 2019. Geophysical Journal International, 219, 2, pp. 1300–1315.
DOI : 10.1093/gji/ggz365

(2) A. Letteron, Y. Hamon, F. Fournier, M. Seranne, P. Pellenard, P. Joseph, 2018. Sedimentary geology, 367, pp. 20-47.
DOI : 10.1016/j.sedgeo.2017.12.023

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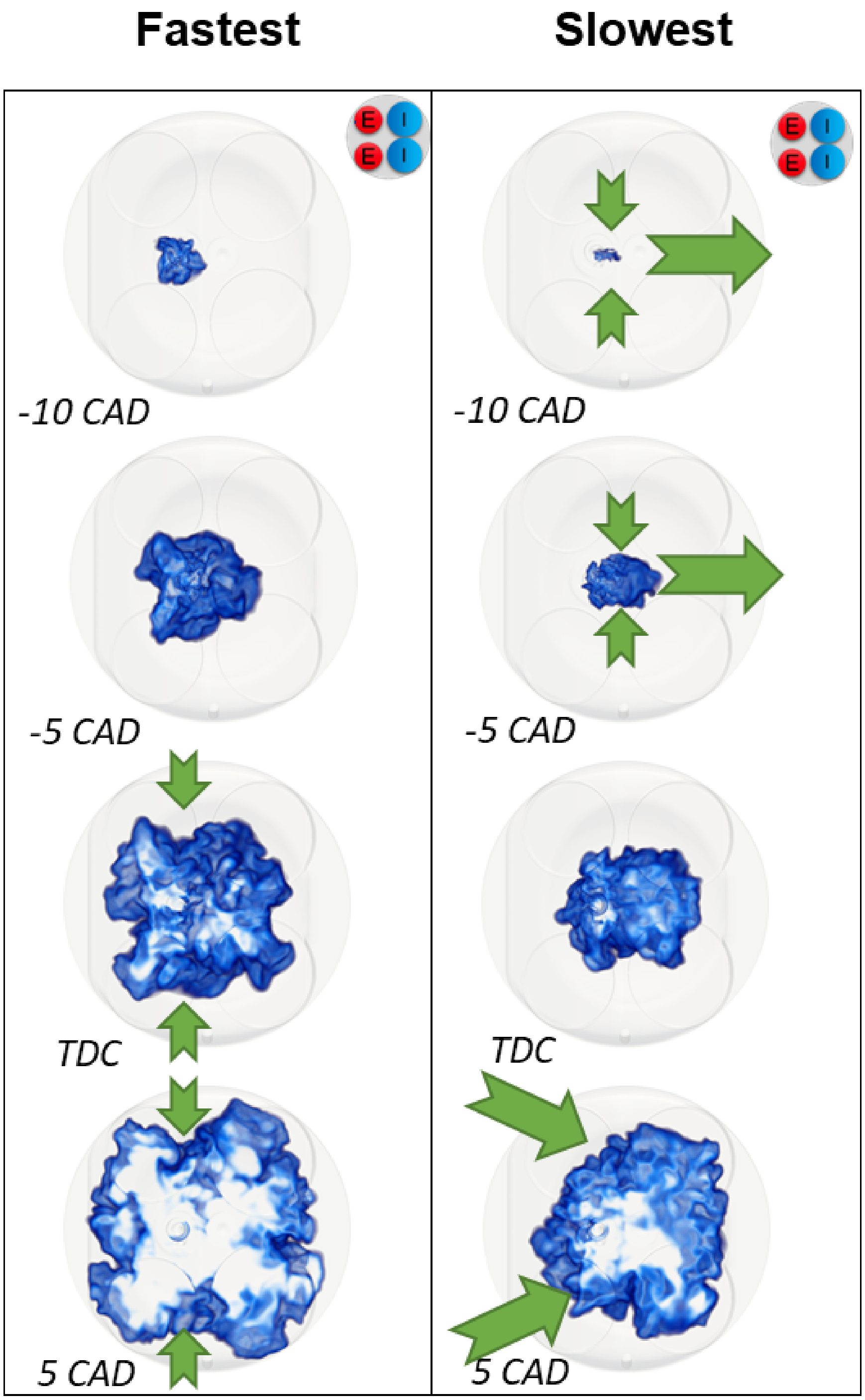
Characterization and modeling of the facies(a)-eogenesis(b) couple, initial state of carbonate reservoirs (HDR 2017)

The scientific field concerned by my HDR research is the 3D numerical modeling of two-phase combustion, combining research on turbulent combustion and the preparation of the reactive mixture.

Building on my PhD, I tackled a number of fundamental questions, such as the modeling of transitions between separated and dispersed phase flows, and the modeling of chemistry/turbulence interactions in stratified media. This enabled me to propose solutions that are now being concretely applied; it is this relationship between theoretical aspects and practical needs that was my area of focus in my HDR.

Today, some models have been integrated in software used in the automotive industry.

The development of a **SaaS (Software as a Service) tool** for **LES (Large-Eddy Simulation)** is an example of how such a transfer can be implemented. The tool is a remote calculation platform providing access to models developed at IFPEN for the **LES of two-phase combustion in engines** (1).



LES calculations for studying acyclisms in spark ignition engines with considerable excess of air in relation to fuel (a)(2).

This tool illustrates how knowledge acquired during PhD research and more fundamental studies is made accessible, greatly facilitating interactions between industry and research.

While remaining within my specialist field, being awarded my HDR enables me to coherently combine the supervision of PhD research with R&I project management activities.

a - Comparisons of flame development for both rapid (Fastest) and slow (Slowest) combustion - TDC: top dead center – CAD: crank angle degree

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(1) A. Robert, K. Truffin, N. Iafrate, S. Jay, O. Colin, C. Angelberger, Int. J. Engine Res., vol. 20, n° 7, p. 765–776.
DOI : 10.1177/1468087418796323, 2018.

(2) O. Benoit, P. Luszcz, Y. Drouvin, T. Kayashima, P. Adomeit, A. Brunn, S. Jay, K. Truffin, C. Angelberger, Technical Paper 2019-01-2209, ISSN : 0148-7191, e-ISSN : 2688-3627, décembre 2019, SAE International

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Multiphase reactive flow simulation: developments and applications in the field of combustion (HDR 2015)

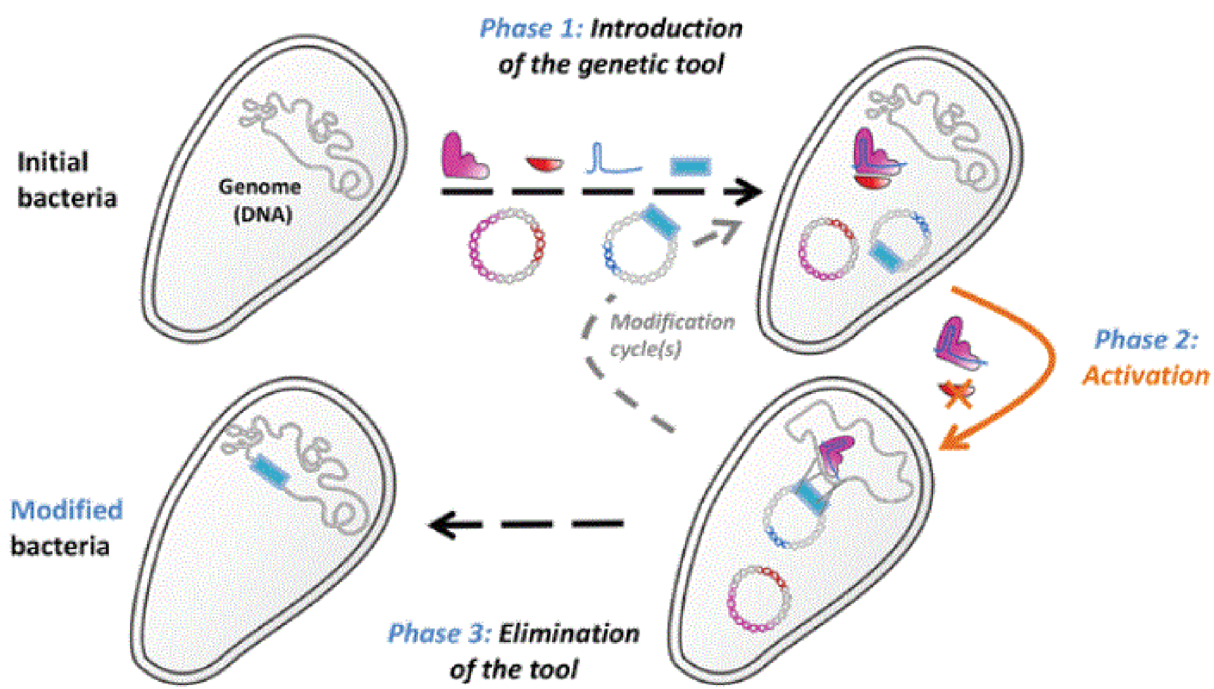
The scope of my HDR covered ten years of research at IFPEN within the context of the **development of Futurol™**, a process aimed at producing 2nd-generation bioethanol from lignocellulosic biomass. My research enabled me to acquire the fundamental knowledge and technical data required to optimize this bioprocess:

• the 1st part was dedicated to the **impact of the physicochemical properties of the biomass of interest**[a] on the performance of the two key steps, i.e. pretreatment and enzymatic hydrolysis;

• the 2nd part led to **the optimization of one key enzyme** contained in the enzyme cocktail produced by the industrial strain Trichoderma reesei fungus;

• the 3rd part concerned the **development of mechanistic or predictive models** for the cellulose hydrolysis step.

Acquiring the HDR allowed me to go on to supervise several PhD theses at IFPEN relating to Futurol™, one of which focused on the “multi-tool characterization” of pretreated biomasses[b].



Diagrammatic representation of the principle underlying IFPEN’s genetic tool based on Crispr-Cas technology.

The experience acquired throughout this period was also invaluable for my contribution to the development of a bio-based industrial solvent production process (n-butanol and isopropanol) using an anaerobic bacteria belonging to the Clostridium genus.

In addition, two theses supervised in partnership with the University of Wageningen resulted in the acquisition of new omic[c] data and the validation of a Crispr-Cas-type genetic tool (figure), currently revolutionizing the genetic engineering of industrial strains (1,2).

a - Including a study dedicated to the modifications produced by the pretreatment step on miscanthus, a rhizome plant being considered as a perennial crop in France
b - Thesis by J. Passicousset: Physicochemical descriptors of lignocellulosic biomass in enzymatic hydrolysis: towards in situ characterization (2019)
c - https://www.ifpenergiesnouvelles.fr/article/chimie-biosourcee-limportance-dacquerir-grand-nombre-donnees-biologiques

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(1) M. Diallo, R. Hocq, F. Collas, G. Chartier, F. Wasels, H. S. Wijaya, M. W. T. Werten, M. W. T. Wolbert, S. W. M. Kengen, J. van der Oost, N. Lopes Ferreira, A. M. López-Contreras (2020), Clostridium beijerinckii. Methods. 172:51-60.

(2) F. Wasels, J. Jean-Marie, F. Collas, A. M. López-Contreras, N. Lopes Ferreira (2017), Journal of microbiological methods. 140:5-11.

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Hydrolysis of lignocellulosic biomass: study of enzyme-substrate interactions (HDR 2015)

My HDR research was aimed at **optimizing catalyst performance using image processing**, automating the analyses and improving the quality of the information extracted from data. The knowledge and tools stemming from my work concern chromatography and X-ray diffraction (1D) signals, electron microscopy (2D) images and electron tomography (3D) analyses.

The latter technique makes it possible **to extract information on a nanometric scale**, the characteristic dimension of mesoporosity in catalyst supports. If provides invaluable information concerning the efficacy and selectivity of catalytic materials via the study of the diameter and connectivity of these pores. These data are useful both for controlling catalyst formulation procedures and improving the understanding of transport phenomena on a mesoporous scale.

Random morphological models (figure) made it possible to reproduce virtual microstructures (numerical 3D) close to those observed and to incorporate slight
geometric modifications (grain size, porosity, etc.) in order to study the impact of these modifications on the textural and usage (diffusion or mechanical) properties. Thanks to this research conducted in partnership with academia[a], the geometric and topological characterization of porous networks has improved via new numerical descriptors of microstructures(1).

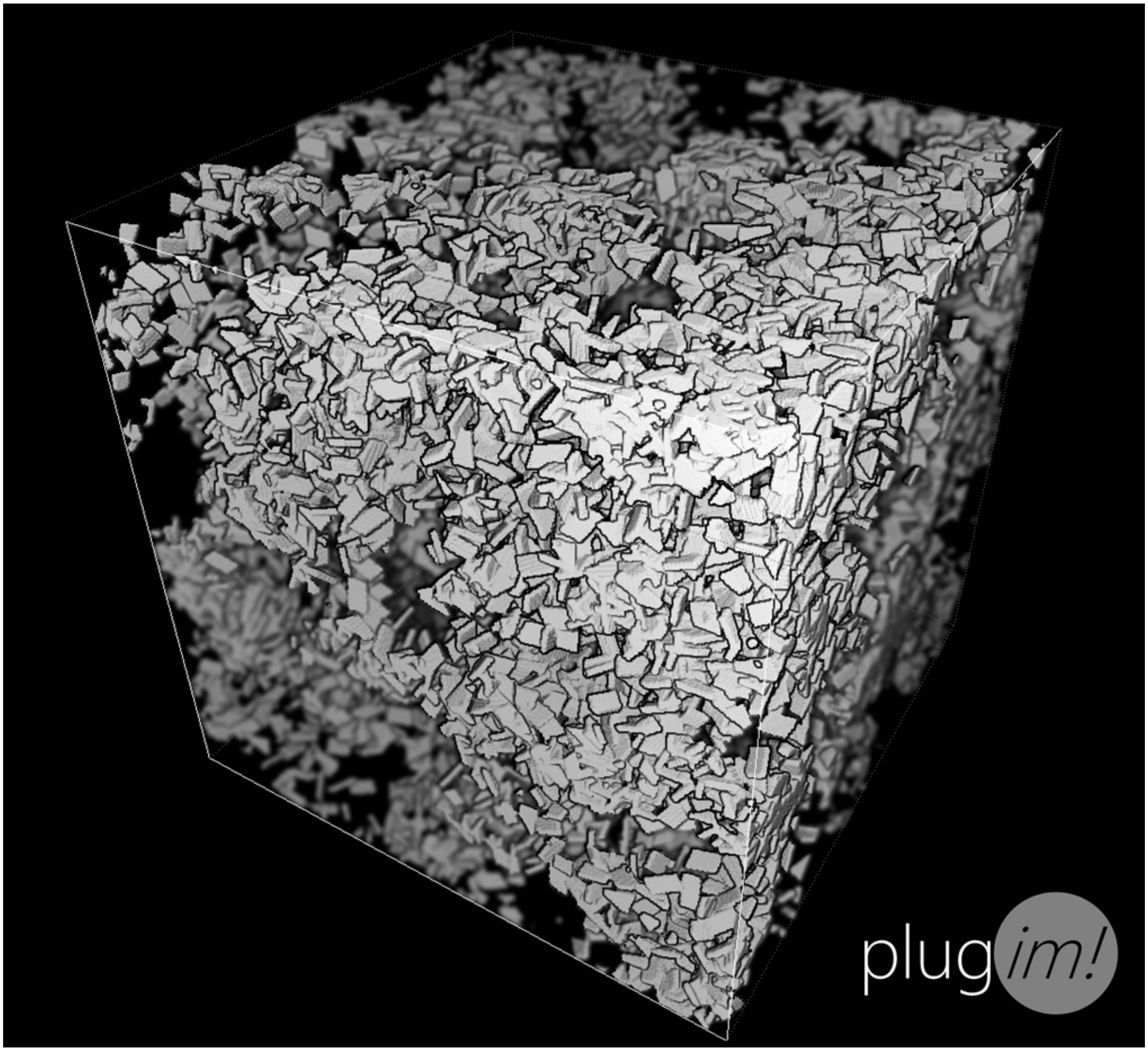

Illustration of a random morphological model
of an alumina microstructure made up of nanoplates.

Available in the plug im! platform (figure), the application of these descriptors used for aluminas(2) has been extended to the field of neurosciences for living cells, in partnership with Laval University's CERVO brain research laboratory in Quebec.

a - Notably the Hubert Curien laboratory at Jean Monnet University and the Mathematical Morphology Center at Mines ParisTech engineering school

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(1) J. Chaniot, M. Moreaud, L. Sorbier, T. Fournel, J. M. Becker, Image Analysis and Stereology 38 (1), p. 25-41 (2019).
https://doi.org/10.5566/ias.2039

(2) A. T. F. Batista, W. Baaziz, A. L. Taleb, J. Chaniot, M. Moreaud, C. Legens, A. Aguilar-Tapia, O. Proux, J. L. Hazemann, F. Diehl, C. Chizallet, A. S. Gay, O. Ersen, P. Raybaud. ACS Catal. 10, p. 4193-4204 (2020).

https://doi.org/10.1021/acscatal.0c00042

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The contribution of image processing to catalyst performance optimization (HDR 2017)

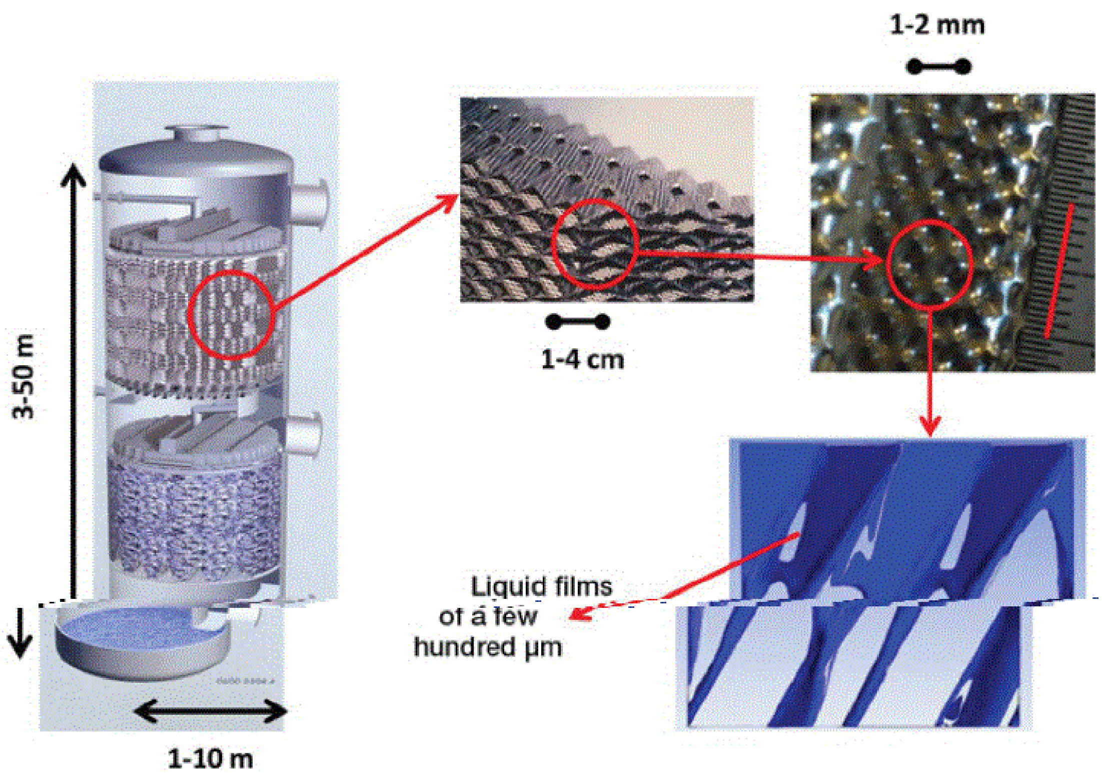
Employed in certain treatment equipment, such as industrial gas purification columns, structured packings are ordered stacks of corrugated metal sheets that promote contact between the gas and a flowing liquid, while minimizing pressure drop.

The developed surfaces of the sheets can be up to hundreds of square meters per unit of volume. The liquid that absorbs and transforms the element to be captured flows through them in the form of laminar films while the gas flow is turbulent. My HDR thesis summarizes research relating to **structured packing columns** that I contributed to.

In order to dimension and optimize facilities, it is necessary to have precise knowledge of packing performance. To this end, **pressure drop**, acceptable gas-liquid flowrates — and mass transfer measurements were taken at IFPEN using various test columns (from 150 mm to 1 m in diameter(1)). Contributions from partner universities supplemented the results obtained.

Knowledge and consideration of multiscale phenomena are necessary **to optimize the choice of packing or to develop new ones** (figure). Research conducted for several theses resulted in the development of flow models (interface monitoring, equivalent porous medium). One such thesis(2) was dedicated to the **sheet wetting mechanism** and to **velocity and local retention acquisition**.

The study of phenomena acting on local flows is continuing in the laboratory but the road ahead is long and experimentation on a scale representative of real equipment remains essential. To this end, the results of all the research mentioned above are currently being used within the framework of an industrial pilot for the H2020 3D project[a].



Multiscale problem of structured packings.

This project, conducted at a steelworks site operated by ArcelorMittal, is aimed at demonstrating the efficacy of the CO_2 capture process using as a liquid a demixing solvent developed as a result of IFPEN research.

a - DMX™ (Demonstration in Dunkirk)

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(1) L. Hegely, J. Roesler, P. Alix, D. Rouzineau, M. Meyer, AICHE Journal, 63(8), 3245-3275, 2017.

(2) Z. Solomenko. Lyon University PhD thesis, 2016.

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Study of packings for natural gas treatment and CO_2 capture columns (HDR 2019)

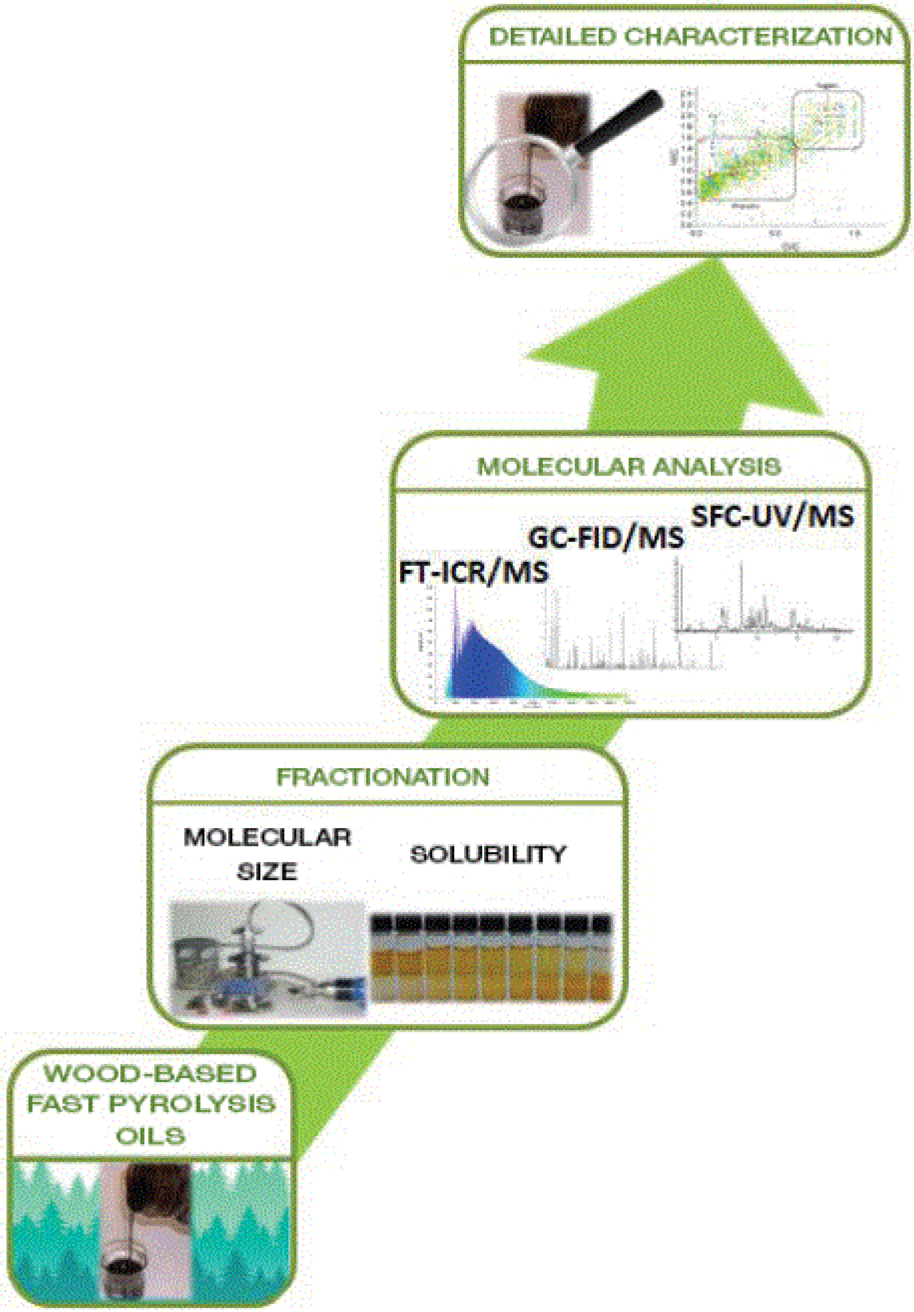
IFPEN offers a broad variety of processes and catalysts for the production of biofuels and bio-based molecules. In order to further develop them, it is necessary **to characterize the key physicochemical properties of the different liquid products** obtained from the lignocellulosic biomass (oxygenated matrices). This is done via **relevant descriptors** that formed the focus of my HDR thesis, as well as several theses I supervised.

The research that gave rise to these descriptors was conducted by several IFPEN divisions working together, in partnership with external players[a].

A multi-technical approach was constructed and adapted depending on the matrix to be characterized, in order to take into account the broad diversity of oxygenated compounds in terms of chemical functions, polarities, molecular masses and concentrations.

The analytical methods developed for the purpose combine **chromatography — gas (GC, GCxGC), supercritical or liquid phase —** as well as **spectroscopy and high-resolution mass spectrometry techniques**. A matrix fractionation step is often carried out prior to the analysis, by volatility (micro-distillation), molecular size (nano-filtration, steric exclusion chromatography) or solubility (centrifugal partition chromatography).

Fast pyrolysis oils, from conifer wood, are the first application of this methodology(1, 2), which made it possible to consider the thermosensitivity, strong polarity and/or high molecular masses of the oxygenated species, in order to achieve a uniquely detailed characterization (figure).



Methodology deployed for the physicochemical analysis of a bio-based liquid.

Originally targeting products derived from the thermochemical conversion (hydroliquefaction, hydrothermal liquefaction, fast pyrolysis) of lignocellulosic biomass or lignin, this analytical strategy has now been extended to new matrices derived through biochemical conversion.

a - a - ESPCI, ICMCB, ICOA, IRCELyon, ISA

(1) A. Dubuis, A. Le Masle, L. Chahen, E. Destandau, N. Charon, J. Chrom. A 1609 (2020)
https://doi.org/10.1016/j.chroma.2019.460505

(2) A. Dubuis, A. Le Masle, L. Chahen, E. Destandau, N. Charon, J. Chrom. A 1597 (2019)
https://doi.org/10.1016/j.chroma.2019.03.031

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Descriptors of oxygenated matrices for lignocellulosic biomass conversion (HDR 2017)

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