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15 minutes of reading

News

Fundamental Research

The use of fundamental research to fuel the technological developments necessary for the energy transition is a core part of IFPEN's roadmap. One of the main challenges that has to be overcome to achieve carbon neutrality by 2050 is the need to obtain even more detailed parametric descriptions of energy production and conversion processes and systems. This requires the gradual replacement of global approaches characterizing the inputs and outputs of these systems with methods based on knowledge of the descriptors governing the detail of the physicochemical mechanisms at play, with the ultimate aim of establishing predictive constitutive laws. In this context, six articles are featured in this issue of science@ifpen.

The first two concern cheminformatics. Firstly applied to managing the compatibility between a polymer and a fluid, an essential aspect when designing a biofuel distribution system. A strong coupling between molecular descriptors and fluid descriptors is introduced in order to construct a set of parameters that can be directly interpreted by machine learning algorithms. These algorithms are also used to identify the chemical properties that control aging by oxidation of new fuels.

The next two articles focus on catalyst optimization. The tortuous paths taken by gases are characterized using digital twins. Catalyst optimization also benefits from the now systematic integration of catalytic descriptors in chemical kinetics models.

In addition, our understanding of the interactions between all the non-linear phenomena associated with turbulence and hydrogen combustion in an IC engine is progressing via the introduction of descriptors based on new modal decompositions of aerodynamic signals from simulations.

Finally, IFPEN is optimizing the prediction of expected coastline changes through the introduction of specific descriptors, combining existing satellite data with information gathered from the field.

I hope you enjoy reading this issue.

Luc Vervisch
Chairman of IFPEN's Scientific Board
Professor at INSA Rouen Normandie
Member of the Institut Universitaire de France

LES BRÈVES

Ensuring compatibility between polymers and fluids is essential in numerous industrial sectors: in the automotive sector, for example, the resistance of materials used in the fuel supply system is a vital consideration. For the components concerned, experimental methods are used to anticipate potential degradation of initial properties. However, these methods remain extremely time-consuming. A more appropriate alternative approach has emerged: use existing data, supplementing it if necessary, to extract information via methods borrowed from data science [1,2].

Cheminformatics lies at the interface of several scientific fields and involves using computer and informational techniques to solve problems related to chemistry. One aspect is the use of artificial intelligence to predict usage properties. In addition to data quality, one of the keys to success resides in the representation of the complex fluids considered, such as the thousands of compounds present in fuels.

Despite constant improvements in analysis techniques, accurately identifying each component of these complex fluids appears to be an insurmountable task. Thanks to two-dimensional chromatography (GC×GC), it is nevertheless possible to quantify the chemical families present and obtain distributions based on the number of carbon atoms. A representative molecule is associated with each component of the distribution: for example, a jet fuel[a] can be structurally represented by a mixture of around one hundred compounds [1].

To ensure it can be interpreted by machine learning algorithms, each of these molecules must be encoded by molecular descriptors. Since these are numerous, the choice was made to use simple descriptors derived from counts of the functional groups present. A descriptor vector encoding the fluid (figure 1) is then obtained thanks to a linear mixing rule applied to the descriptors, the components and their respective fractions.

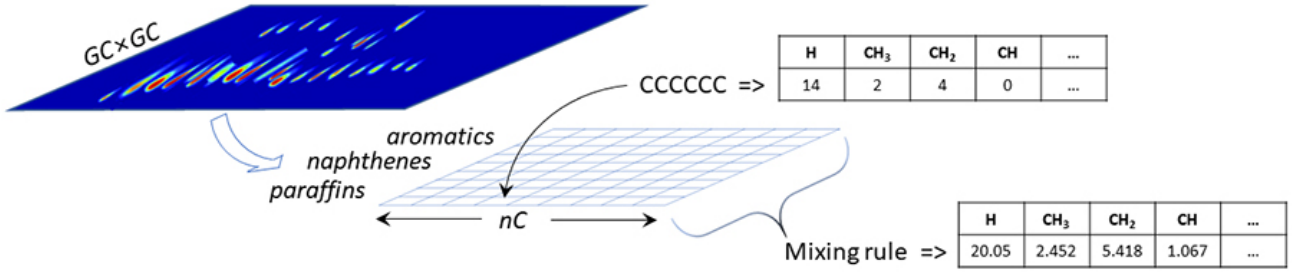

Figure 1: Description of a complex fluid to feed into machine learning algorithms.

This methodology has been used to model the quantity of fluid penetrating a polymer when the two come into contact with each other. Different polymer/fluid combinations have thus been studied, databases created and machine learning algorithms applied.

The models obtained make it possible to instantly anticipate the impact of adding biofuels to gasolines, or the use of alternative jet fuels on the properties of various polymers (figure 2).

Such a modeling approach helps to significantly reduce the time required to quantify polymer/fluid compatibility.

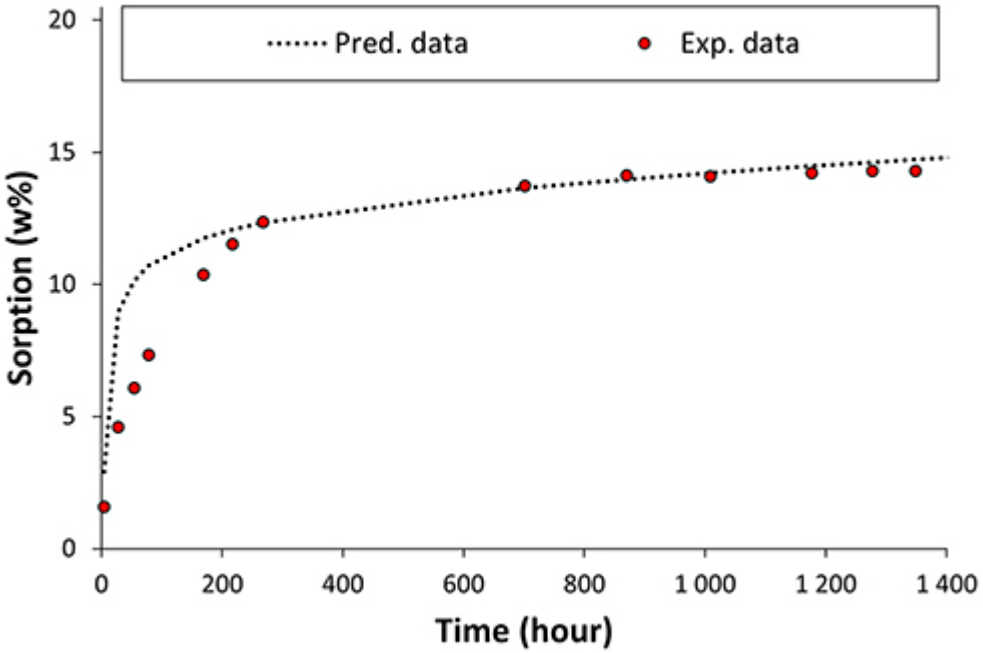

Figure 2: Capacity of models to predict the quantity of jet fuel penetrating a polymer (case of NBR , Nitrile Butadiene Rubber).

In the context of the representation of complex fluids, at least two types of developments can be envisaged:

- integration of the in silico generation of structures [3] to obtain an even more detailed characterization;
- the application of this modeling methodology to the modeling of other phenomena, such as fluid aging, for example.

a- or kerosene
b- Material used in fuel circuits: tanks, pipes, gaskets

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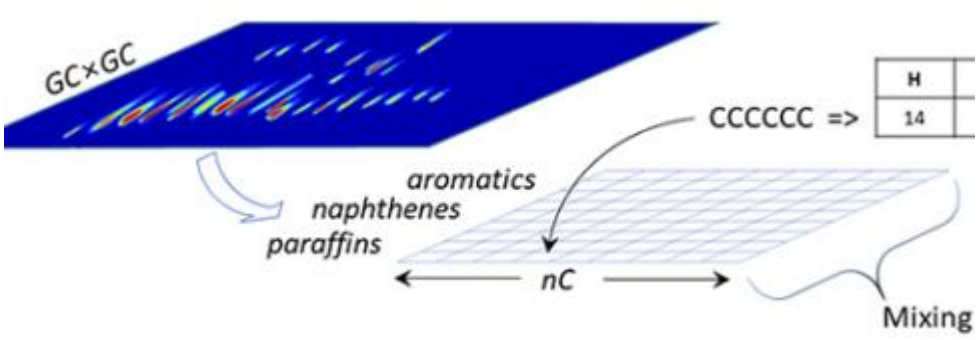
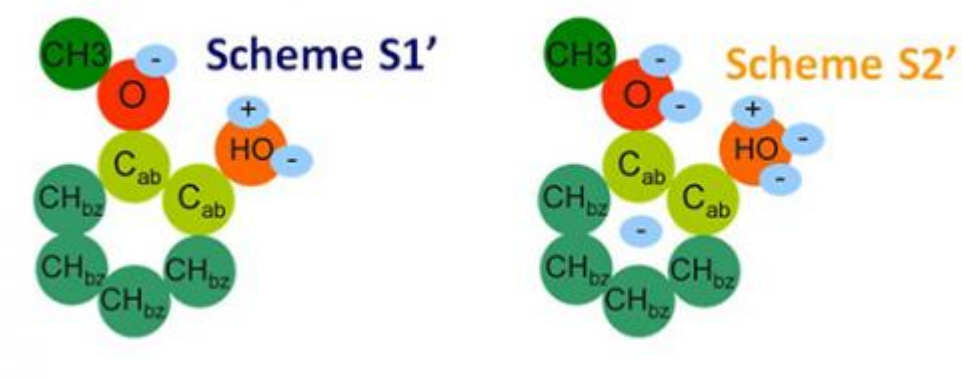


Cheminformatics and its descriptors: application to polymer/fluid compatibility

Ensuring compatibility between polymers and fluids is essential in numerous industrial sectors: in the automotive sector, for example, the resistance of materials used in the fuel supply system is a vital consideration.

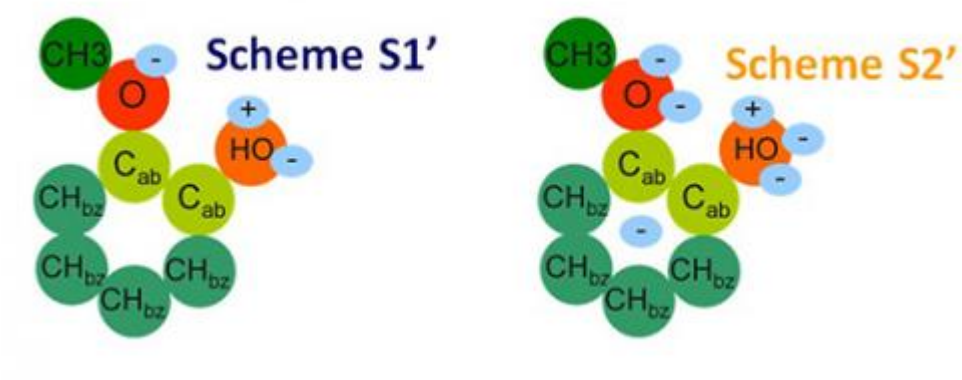
Chemical analysis | **Thermodynamics/Molecular modeling** | **Signal processing/Data science**



Review of a Chair on “thermodynamics for biomass fuels”

Unlike hydrocarbons of fossil origin, the molecules derived from biomass are polar, due to the heteroatoms they contain. This difference on a molecular scale induces a more complex macroscopic behavior that must be taken into account when designing the processes where such mixtures are encountered.

Physical Sciences | **Thermodynamics/Molecular modeling**



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Physical Sciences | **Thermodynamics/Molecular modeling**

Cheminformatics and its descriptors: application to polymer/fluid compatibility

IFPEN uses numerous fluids in its fields of innovation for a variety of applications, ranging from renewable energy production to sustainable mobility. Many of the fluids are complex mixtures and the chemistry of their components (hydrocarbons, alcohols, esters, etc.) varies depending on the target application: combustion, cooling, lubrication, electrical insulation, etc. Irrespective of the application, it is vital that the products in question retain all their properties over time, hence the crucial importance of their stability. In this respect, degradation as a result of oxidation is one of the phenomena liable to alter the quality of certain fluids and thus reduce the efficiency of the system employing them, sometimes to the point of system failure.

In this context, a research project, launched in partnership with Lille University, is hosting a PhD thesis [a] focusing on the issue of fluid reactivity. The aim is to identify the key physical and chemical characteristics for predicting their oxidation stability. To do so, an original approach is being used based on the establishment of global models (figure) comparing and combining two supervised machine learning approaches already successfully employed independently at IFPEN:

- Cheminformatics and principally the development of QSPR (Quantitative Structure Property Relationship) models. These multivariate models provide property values using fluid structure and molecular compositions as input data [1];
- Chemometrics and, more specifically, the development of models based on mid-infrared (MIR) spectroscopy or near infrared spectroscopy (NIRS) These multivariate models, often developed based on “components” (PCA[b], PLS[c]), associate properties of interest with vibrational bands characteristic of the fluids analyzed [2].

By analyzing the information extracted from these two types of representation, it will be possible to construct new models. Capable of describing and predicting fluid stability, they will contribute to:

- the development of new formulations to take into account future constraints linked to new usages, and even the identification of new product sectors, within the context of the energy transition;
- the prediction of fluid reactivity in real operating conditions, with a view to proposing improvement solutions.

The idea then is for these models to be implemented in numerical simulation tools, such as the ReFGen[d] thermodynamic property estimation software for “Transport” applications.

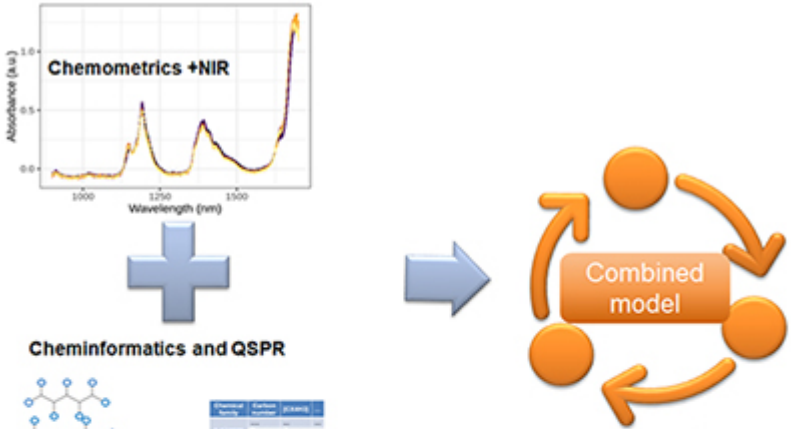

Figure: Illustration of the development and validation of new fluid stability prediction models.

a- Thesis title: “Investigation of descriptors for the understanding and prediction of fluid oxidation stability by via machine learning”, by Adrian Venegas Reynoso
b- Principal component analysis
c- “Partial least squares” method
d- Representative Fuel Generator

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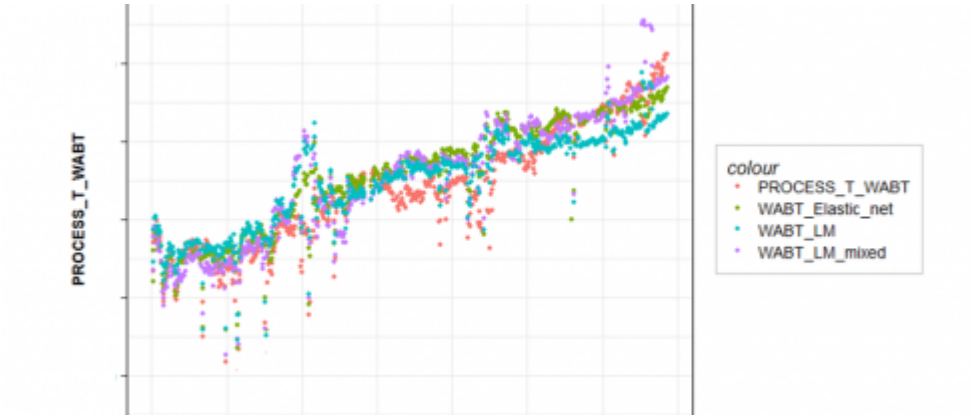

Mix between kinetic and machine learning models

Having access to increasingly precise and robust extrapolation models to be able to predict certain properties[a] remains a major challenge for chemical processes industry.

Engineering sciences | **Fluid mechanics** | **Chemical engineering and process engineering**
Systems modeling and simulation | **Mathematics and IT** | **Numerical methods and optimization**

Fundamental Research

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Analysis and characterization | Chemical analysis

Prediction of fluid oxidation stability via machine learning

In catalytic processes, an active phase is necessary to accelerate the transformation of the molecules in the fluid treated. Most of the time, this catalytic agent is placed on a porous support with a large internal surface area, making it possible to host a large number of active sites within a small volume. However, in addition to the quality and activity of the active phase, the performance of a catalyst is also determined by the accessibility of these reaction sites to the molecules contained in the fluid. Improving catalyst performance thus depends on a good description of effective molecular diffusion within the porous support, which itself requires a better understanding of the internal topology of said support.

The porosity of a material is usually characterized by means of a nitrogen adsorption and desorption technique. However, this method only provides indirect information relating to the porous support's topology and architecture. An *in silico* representation of this material can nevertheless be obtained by creating a digital twin using a network of pores. This digital equivalent is therefore a model that is very useful for understanding how the textural properties and topology of the network influence the diffusion of molecules through the porosity[a].

In order to produce this model, algorithms were developed to create a three-dimensional network of interconnected cylindrical pores, the characteristics of which are obtained via Monte Carlo sampling of parametrized distributions [1]. From the resulting network, it is possible to numerically simulate nitrogen adsorption and desorption or mercury intrusion porosimetry curves using dedicated algorithms, based on the theory of invasion percolation. Model parameters are then adjusted via the calibration of this simulated data with experimental measurements, making it possible to adapt the pore network to the structure of various real solids.

The digital twin obtained was validated via the calculation of its tortuosity factor, by simulating the diffusion of a tracer in the pore network. Comparison to the experimental tortuosity factor, measured by pulsed field gradient NMR on a physical sample, enabled validation of the approach [2].

In summary, the detailed representation of a porous structure, obtained using numerical tools and widely available experimental data, makes it possible to extract topological information for a reasonable cost. In the case of a catalyst support, it is thus possible to reproduce the tortuous paths molecules have to follow in order to reach the active phase. The use of this type of model will ultimately steer research towards optimized materials from the point of view of their porosity, using diffusion-reaction simulations for different reaction systems.

Figure: Representative Elementary Volume of the digital twin of a real alumina.

a- This research was conducted within the framework of Gabriel Alejandro Ledezma Lopez' thesis entitled "*Suitable Representations of Gamma Alumina Porous Structures by Computational Modeling*", supervised by Christian Jallut from Claude Bernard Lyon 1 University..

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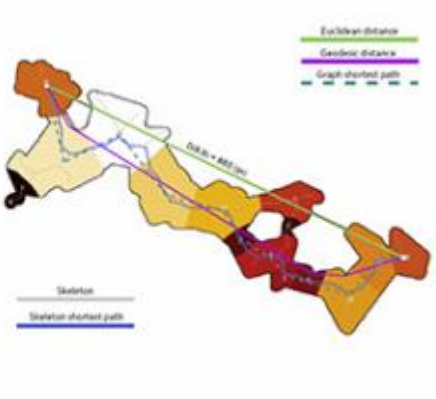
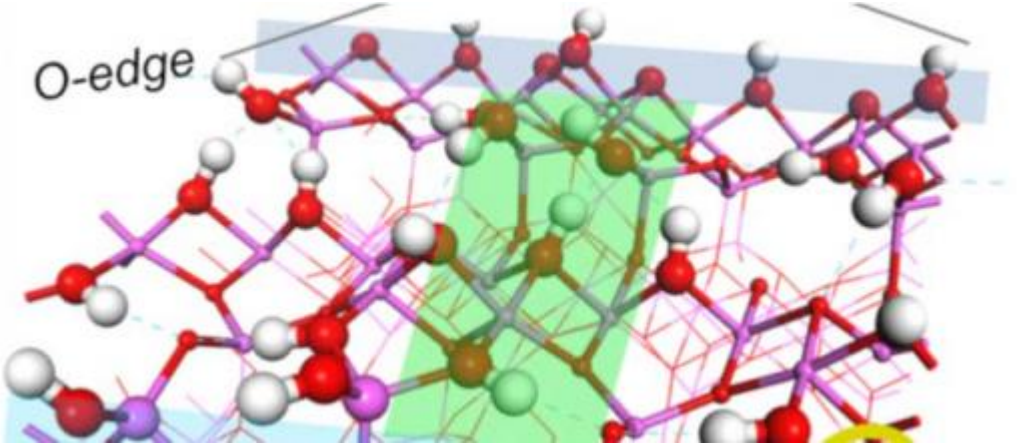


Numerical design based on the analysis of multi-scale porous material microstructures

The design of high-quality porous materials is a major challenge for the energy efficiency of industrial processes in the fields of catalysis and biocatalysis and separation and purification operations. For such applications, these materials derive their properties of interest from their specific microstructure, incorporating a large quantity of empty spaces that are organized and connected on a nanometric scale. IFPEN and Saint Gobain Research Provence (SGRP) joined forces to acquire a tool that will ultimately facilitate the development of porous materials optimized for given usages.

Analysis and characterization | Structural analysis and Imaging | Physical chemistry | Surface, interface and materials science | Mathematics and IT | Signal processing/Data science



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Spectroscopy and quantum calculations uncover the secrets of alumina supports

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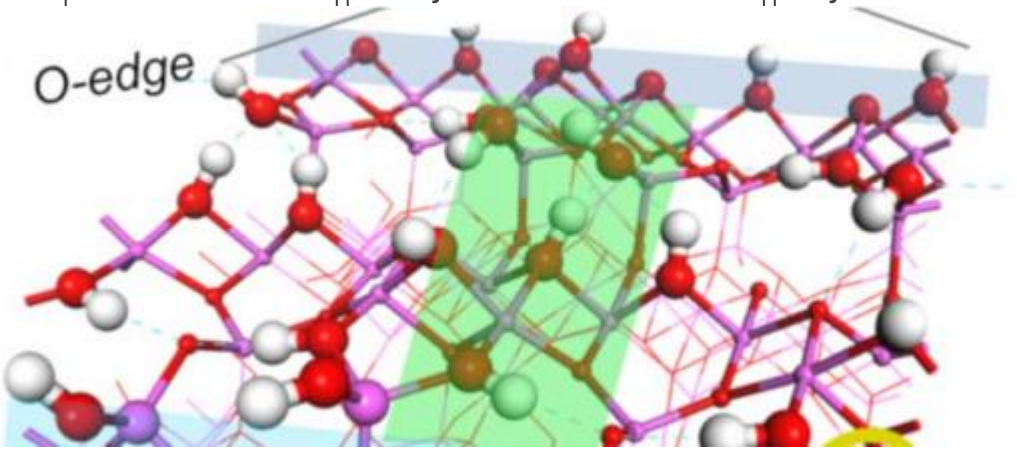

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Spectroscopy and quantum calculations uncover the secrets of alumina supports

Chemical sciences | Catalysis and reaction kinetics | Physical Sciences | Thermodynamics/Molecular modeling | Physical chemistry | Surface, interface and materials science

Diffusion in catalysts: an often tortuous path!

The vast majority of oil refineries are equipped with a catalytic reforming unit that fulfils three main functions: production of high-octane oil cuts for gasoline production (known as reformates), production of aromatic-rich cuts containing fewer than 10 carbon atoms, used in the chemicals industry, and generation of dihydrogen, primarily used in hydrotreatment and hydrocracking units.

For naphtha[a] reforming units , a close but non-rationalized link connects the distribution of products exiting the process, and hence selectivity, to the formulation of the active catalyst phase. One of the solutions under consideration to provide a better understanding of this link involves developing kinetic models capable of integrating some of the catalyst's physicochemical properties (catalytic descriptors) as input parameters.

The integration of these catalytic descriptors in kinetic models would then make it possible to better anticipate the effect of active phase changes on the catalytic performance of processes but also to propose innovative formulations to maximize catalyst selectivity.

For this purpose, a PhD project[b] focused on describing the links between a catalyst's selectivity and its formulation. This project studied the bi-functionality of the catalyst (Pt/Al_2O_3-Cl) used for the naphtha reforming reaction. This case is complex since certain reactions only take place on acid sites created by the presence of Cl, others on metal - Pt - sites and others still require the presence of both sites, with, in this case, the influence of distance on catalyst selectivity. The challenge with this research lay in the identification of easily quantifiable, controllable and adjustable selectivity descriptors.

A kinetic study of this reaction for n-heptane was conducted for 24 catalysts, covering various platinum and chlorine concentrations, and using different supports, in order to vary the descriptors of both the acid (Cl content, Pt-Cl distance) and metal (Pt content) phases. This experimental study was conducted for each catalyst in an HTE unit[c]. The kinetic constants for each catalyst were first estimated via a power law model and then correlated with the descriptors.

The results obtained shed light on the catalyst formulation/selectivity relationship and reveal hitherto unexpected phenomena concerning the effect of chlorine on the metal activity of platinum particles [1,2]. In particular, surprising results were obtained concerning hydrogenolysis reactivity[d] (figure):

- a preferential activity on one of the catalyst supports, with a minimum of activity at intermediate chlorine concentrations;
- a link between activity and chlorine concentration.

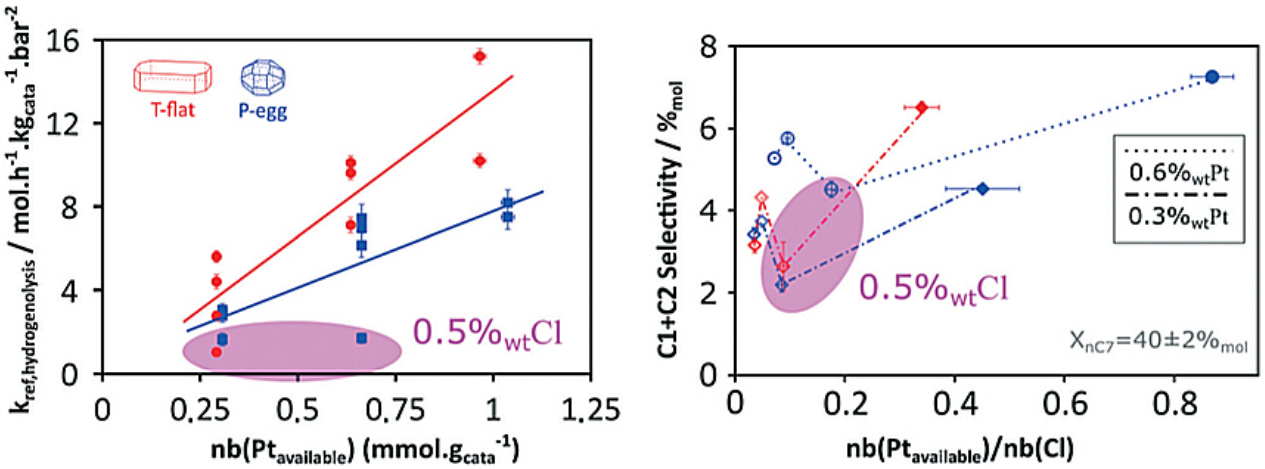

Figure: Effect of the support and chorine inhibition, at intermediate concentrations (0.5%wt) on the hydrogenolysis kinetic constant (left) and selectivity (right).

By combining the modeling approach with high-throughput experimentation and the use of sophisticated characterization methods (proton NMR, H_2/O_2 assays, HR-TEM, *ab initio* calculations and XAS), this research resulted in significant progress towards the development of kinetic models for reforming. These models integrate catalytic descriptors as input data. The research also highlighted unexpected behaviors that will be exploited as potential avenues for innovation in the development of new catalysts.

The task now is to extrapolate the findings to actual reforming feeds and optimize characterization of the active catalyst phase, via a model reaction adapted to mild acidic supports.

a- Liquid light hydrocarbon mixture obtained from crude oil distillation
b- Thesis title: “Identification of active phase catalytic descriptors in the reforming of n-heptane”
c- High-throughput experimentation
d- Chemical reaction whereby a covalent carbon-carbon bond or carbon-heteroatom single bond is cleaved by hydrogen

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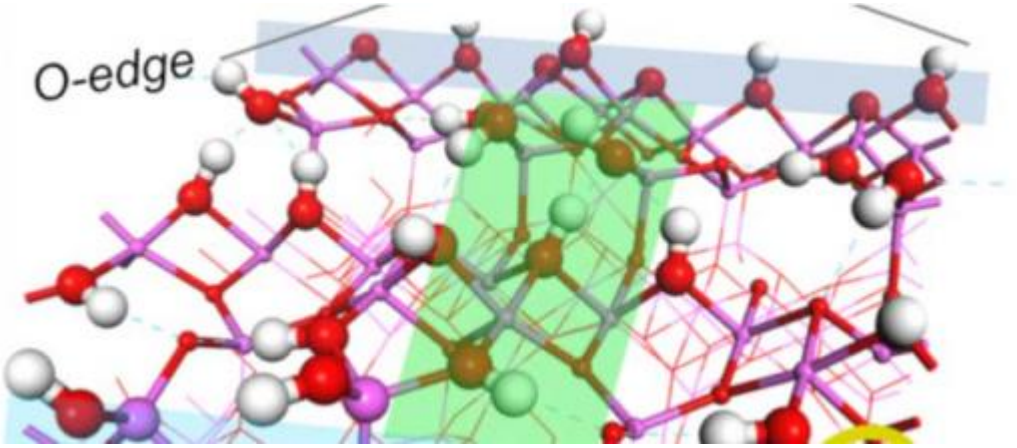

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Spectroscopy and quantum calculations uncover the secrets of alumina supports

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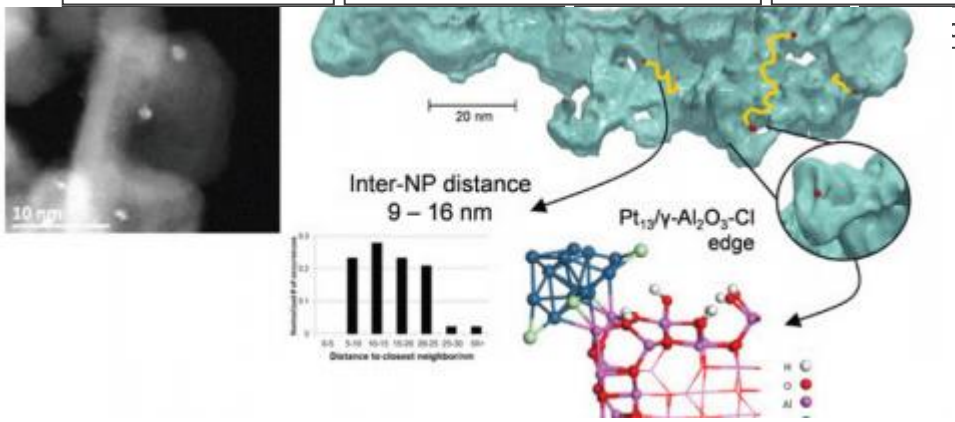

Metal nanoparticles living on the edge

Platinum nanoparticles supported on chlorinated ?-alumina are used in bifunctional heterogeneous catalysts, which are central to numerous industrial processes. An atomic-scale study...

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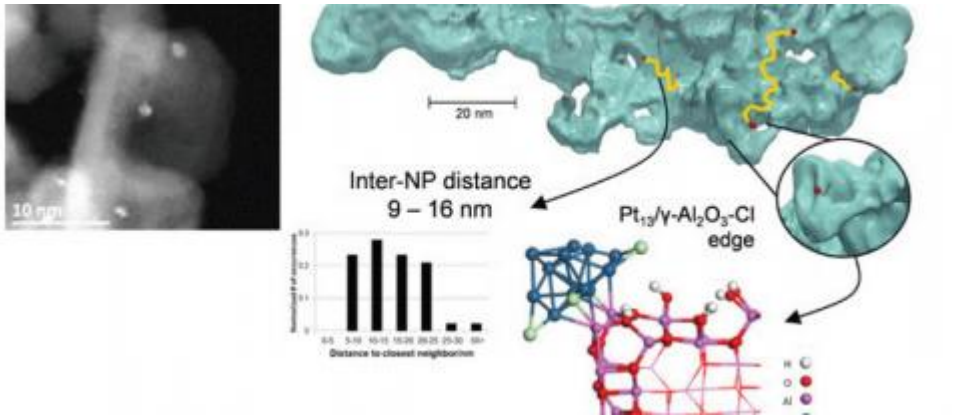

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Chemical sciences | **Catalysis and reaction kinetics** | **Organic and mineral synthesis** | **Analysis and characterization** | **Structural analysis and Imaging** | **Physical Sciences** | **Thermodynamics/Molecular modeling**

Identification of reforming active phase catalytic descriptors

Within the framework of a global policy to reduce the emissions produced by the transport sector - particularly road transport - IFPEN is focusing on a complementary option along with vehicle electrification: the use of hydrogen powertrains. However, the use of hydrogen in IC engines first requires a comprehensive understanding of different phenomena, associated, for example, with interactions between the fuel and air. This objective requires advanced modelling tools for the simulation of turbulent reactive flows, as well as dedicated numerical methods making it possible to fully exploit the results obtained.

In this context, Large-Eddy Simulation (LES) is used to realistically reproduce turbulence, thanks to a detailed description of the vortices and particularly acyclical phenomena [1]. However, access to this non-stationary data is not immediate; it requires adapted tools, capable of identifying two types of movements that are potentially the source of the cycle-to-cycle variabilities observed in an engine: the movement of the flow as a whole and the fluctuating movement associated with turbulence.

The method used for this purpose was EMD (Empirical Mode Decomposition), making it possible to effectively isolate the low-frequency and high-frequency components of a signal. Initially developed in 1D, it was extended to 2D for engine applications [2], and then 3D within the framework of a thesis project [3,4]. Its advantages are that it only uses one velocity field for calculations, unlike traditional approaches such as POD (Proper Orthogonal Decomposition), and does not require criteria to isolate the two components, unlike wavelet-type or Gaussian-filter approaches.

Accordingly, via the use of 3D EMD, it is now possible to consider any velocity field during an engine cycle and have access to the variability of major vortex structures between cycles. This is a significant contribution in terms of the analysis and understanding of the physical mechanisms leading to cyclical combustion variabilities. It also makes it possible to define descriptors specific to the high- and low-frequency components of the velocity field, as well as their variability (figure). The impact of different phenomena (valve jets, interaction between walls, tumble movement[a], gas injection) thus becomes measurable.

This research led to the development of an innovative technique for defining new turbulent flow descriptors in highly unsteady situations, such as those encountered in hydrogen engines. This technique paves the way for even more in-depth analyses of turbulent aerodynamics, with a view to identifying the mechanisms responsible for certain undesirable phenomena (noise, emissions, etc.) affecting other energy conversion solutions, such as electric machines or wind turbines.

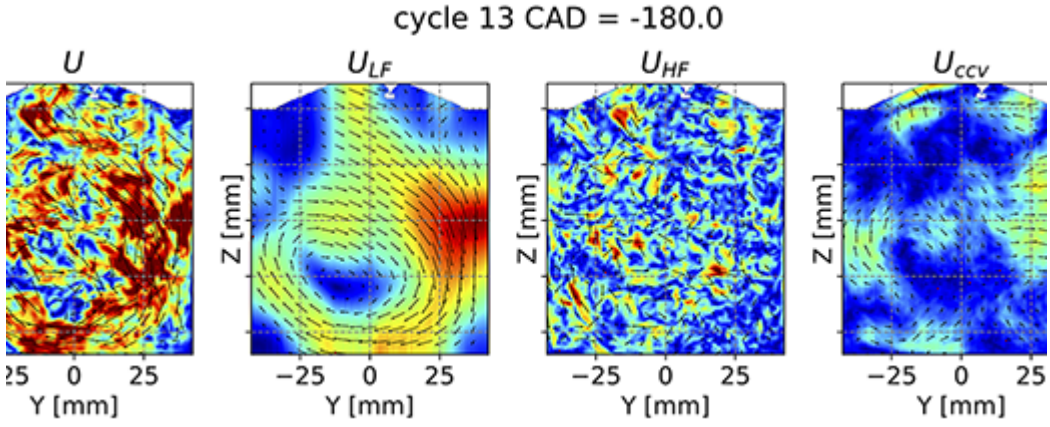

Figure: EMD of a turbulent velocity field derived from LES calculation (2D cut). From left to right: instant velocity field U, its low-frequency component ULF, its high-frequency component UHF, speed variability compared to the average of the whole UCCV.

a- Rotational aerodynamic movement around an axis perpendicular to the axis of the piston motion.

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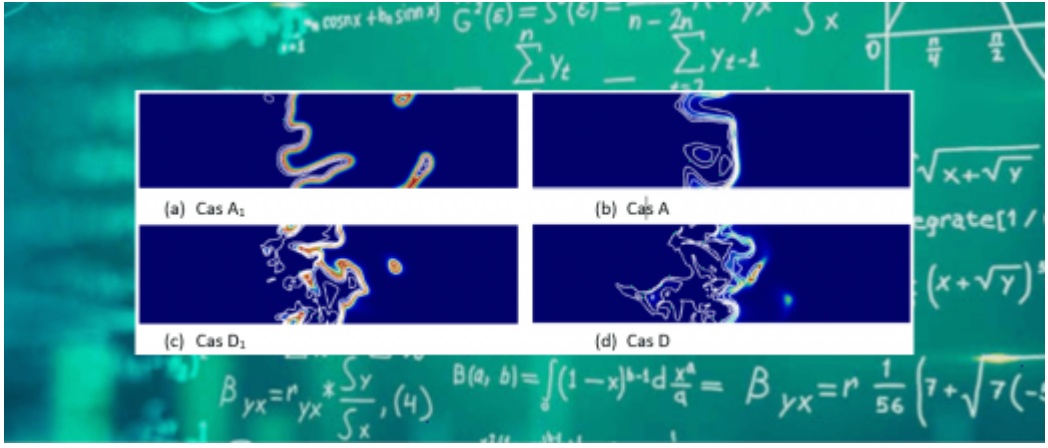

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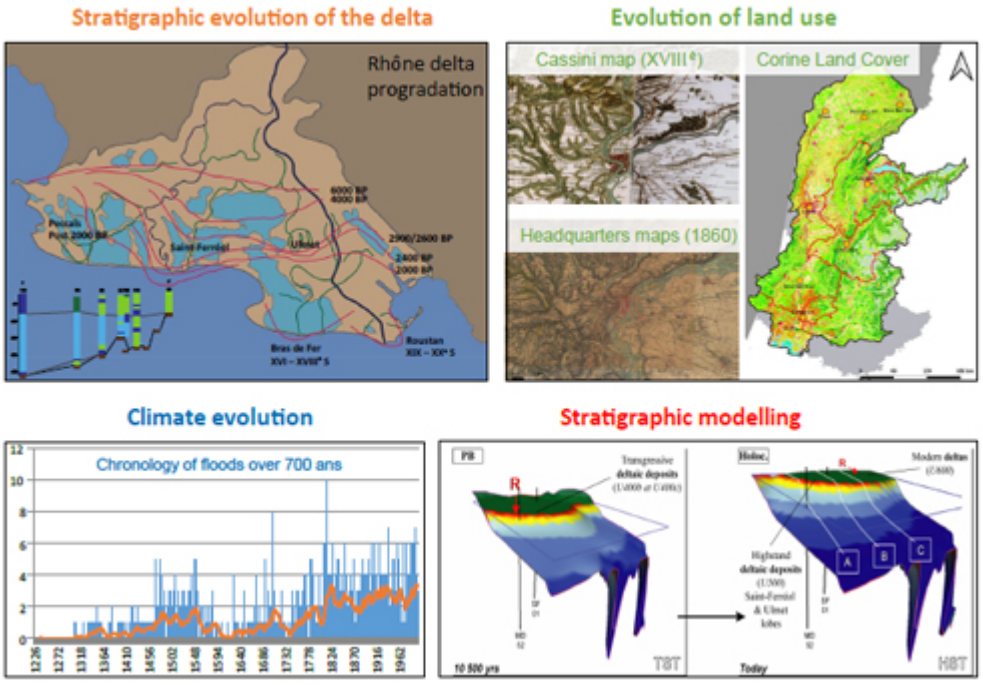
A better description of turbulent flows for hydrogen powertrains

Coastal sedimentary basins evolve under the effect of interactions between, on the one hand, hydroclimatic processes taking place in catchment areas, and on the other hand coastal marine processes that remodel the coastline. The evolution of these environments is naturally controlled by the climate, over different time periods (ranging from tens of years to thousands of years), through variations in sedimentary flows and erosion, which alter the terrain. Another more recent factor controlling geomorphological evolution which has an extremely significant impact is human activity. Anthropism has considerably modified the natural environment impacting resource management (aquifers) and regional planning (river bank instability, flood management, etc.).

In order to predict the impact of various environmental changes scenarii, and thus enable the planification of appropriate local policies, it is essential to have access to modeling tools capable of integrating these different aspects. This requires the development of numerical models that enable to integrate the factors driving changes in the natural environment. Such models must then be parametrized, and the main challenge here is to quantify the different controlling factors and their impacts on the environment over various periods of time.

The Rhône delta, and more particularly its evolution since the quaternary glaciation period, is the ideal laboratory for studying human/habitat interactions and their impacts on the environment. The stratigraphic evolution of the Rhône delta is extremely well documented through numerous sedimentary archives accessible both on the delta plain and in the marine area of the delta, as well as in the catchment area. Moreover, the numerical interpretation of old maps [1-3] and satellite data enable to unravel the evolution of land use, which can then be used as a basis for determining erosion potential and particle flows transported to the delta. The analysis of all this data (figure) will help at calibrating stratigraphic models of the delta's past evolution, using DionisosFlow^{TM} software. On this basis, it will be possible to propose predictive scenarii for the delta system evolution.

This approach, aiming at correlating the evolution of the Rhône catchment area with the delta's sedimentary dynamic is being implemented within the framework of a PhD thesis[a] in partnership with Lumière Lyon 2 University and the Rhône Sediments Observatory (OSR).



Integration strategy: 1- sedimentary information for the delta,
2- volumes of sediments eroded in the catchment area (indirectly quantified based on the evolution of land use),
3- climatic evolution, in order to
4- calibrate a stratigraphic modeling approach.

a- Thesis title: “Impact of hydroclimatic and anthropological parameters on sedimentary dynamics. Rhône delta system in the Holocene-Anthropocene transition”.

References:

1. Martinez, T., Hammoumi, A., Ducret, G., Moreau, M., Berger, J.F., Deschamps, R., 2022. **Semantic multi-class segmentation of the Cassini land use map (XVIIIth c.): the first step of a geomorphological comparative studies**. Article submitted to Computer geosciences

2. Martinez, T., Deschamps, R., Ducret, G., Berger, J.F., Hammoumi, A., Moreau, M., Jouet, G., Piégay, H., Vella, C., 2022. **Fluvial geomorphology, sedimentology and cartography supporting spatio-temporal modelling of the large Rhodanian catchment area**. Paper presented at the Quaternaire 13 conference, Strasbourg 14-18 March 2022

3. Martinez, T., Hammoumi, A., Ducret, G., Moreau, M., Berger, J.F., Deschamps, R., 2022. **Inputs and application of an automated multi-class segmentation of the Cassini land use map (XVIIIth c.) to the understanding of landscape and river dynamics at the end of the LIA**. Extended abstract at IS Rivers congress, Lyon 4-8 July 2022

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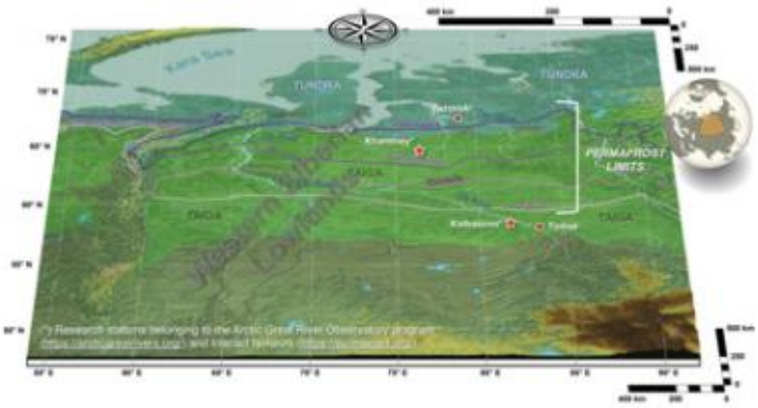

Global change, impact on landscapes and water resources

Today, the impact of climate change and human activities on the evolution of landscapes and water resources is a major challenge. Predicting it requires dedicated tools capable of evaluating, 100 years ahead, the consequences of different scenarios on watersheds and groundwater. To this end, IFPEN is developing modeling approaches targeting erosion-transport-deposition phenomena combined with surface and subsurface flows. ...

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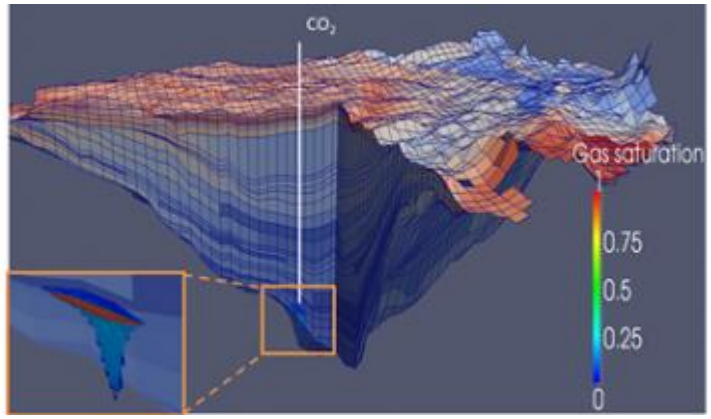

Underground modeling: an essential step for the energy transition

To address the challenges of the energy transition, the subsurface has an important role to play, both in terms of providing resources and offering storage solutions. (...) Numerical models can help gain a better understanding of the subsurface with a view to its long-term management and optimal use. Developed for a number of years now at IFPEN, initially for the petroleum industry, such models cover scales ranging from the sedimentary basin to the reservoir...

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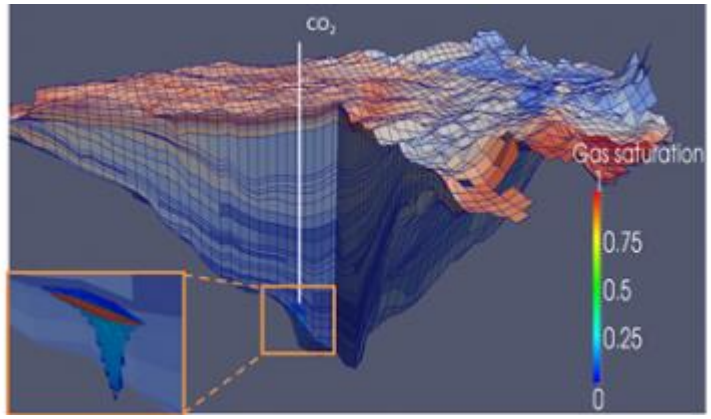

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Impact of hydroclimatic and anthropological parameters on the dynamics of the Rhône delta

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