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News

Fundamental Research

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Whether in our smartphones or in the context of the energy transition, batteries already play a key role in our daily lives. They are complex “objects”, comprising compartments, components, electrolytes and multiple interfaces that enable reversible energy storage.

Like any object, batteries wear out. In doing so, they suffer a gradual loss of their storage capacity. In the case of lithium batteries, one of the aging mechanisms is linked to the formation of an ultra-thin layer (about one nanometer), which forms at the interface between the anode and the electrolyte. This layer, known as a Solid Electrolyte Interphase (SEI), grows over time, consuming the cyclable lithium and ultimately leading toa loss of capacity.

In order to increase the life-span of batteries, it is important to understand the origin of their life cycle and the growth mechanism of this ultra-thin layer. Given the complexity of ageing phenomena and the difficulties involved in characterizing them, one possible approach is modelling. That was the focus for the research conducted by Mohammed BIN JASSAR for his PhD thesis. In particular, he obtained an atomistic description of the decomposition of the electrolyte and a description of the growth of the SEI and associated loss of capacity. The evaluation of several calculation approaches enabled him to increase the efficiency of the simulations and to demonstrate the current limits of these approaches.

This thesis is a perfect illustration of the kind of doctoral work carried out at IFPEN, i.e., of excellent scientific quality while tackling concrete problems and issues of relevance to our lifestyles. It lays a solid foundation for understanding the aging mechanism of batteries, a first step towards predictive models and, ultimately the improvement of our daily lives. This is the reason why Mohammed has been awarded the 2024 IFPEN Yves Chauvin thesis prize.

We hope that you enjoy this issue.

LES BRÈVES

Thesis by **Mohammed Bin Jassar, winner of the 2024 Yves Chauvin prize**: « ***Mieux comprendre la formation et la croissance de la Solid Electrolyte Interphase dans les batteries Li-ion par une approche de modélisation moléculaire*** » **(Gaining a better understanding of the formation and growth of the Solid Electrolyte Interphase in Li-ion batteries via a molecular modeling approach).**

The gradual loss of autonomy of lithium-ion batteries, used in our cell phones and electric vehicles, is notably linked to the formation of a layer known as a Solid Electrolyte Interphase (SEI), which builds up between one of the electrodes and the battery electrolyte. The formation of this SEI layer (Figure 1) was studied theoretically in this thesis using molecular modeling to improve the understanding of its thermodynamic and kinetic aspects.

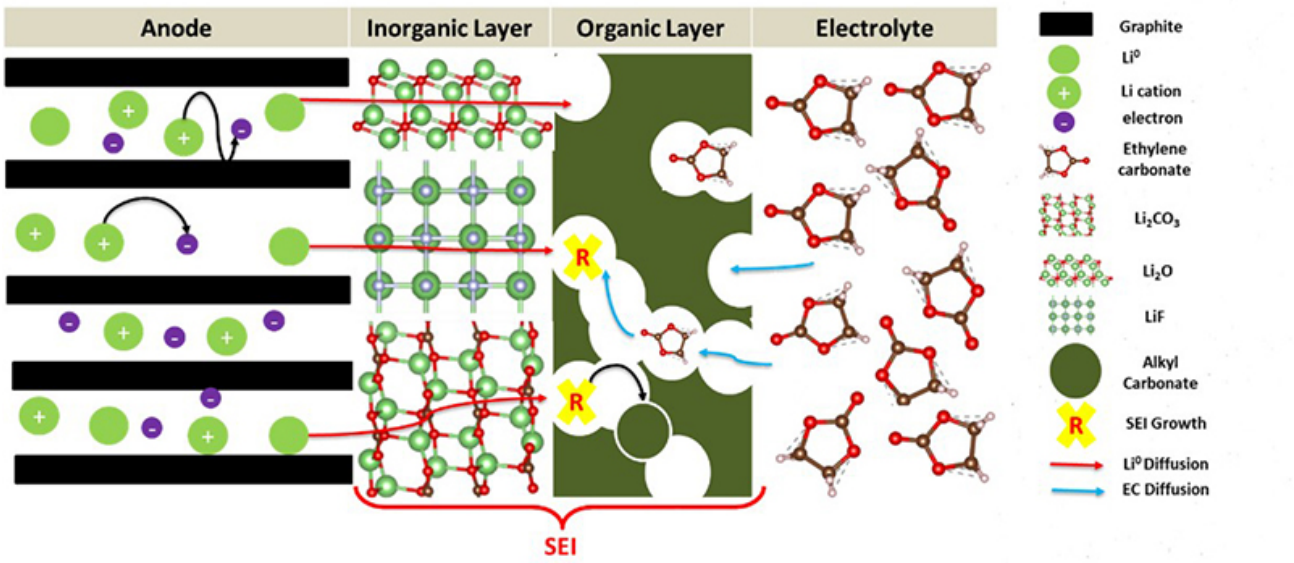

Figure 1: lustration of the graphite/lithium anode,
and the inorganic and organic layers forming the SEI layer and the electrolyte.

The PhD research initially focused on compiling a database of the principal degradation reactions involved by calculating the reaction and activation energies using DFT[1]. The results used in KMC[2] simulations then revealed that salts such as Li_2CO_3 and Li2O, derived from electrolyte degradation, play a crucial role. Simulations are also used to predict the loss of battery capacity as a function of the initial composition of the SEI layer (Figure 2) and hint the importance of considering other salts such as LiF resulting from degradation [1].

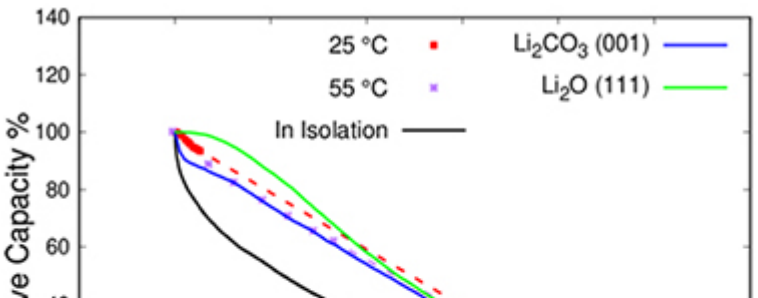

Figure 2: Decrease in relative capacity as a function of normalized time following electrolyte degradation reactions in the presence of Li2CO3 (blue curve), Li2O (green curve) and in the absence of inorganic salt (black curve), compared with experimental data obtained at 25°C for a 100% charged battery [2] and at 55°C for a 60% charged battery [3].
(Reprinted with permission from [1] - Copyright 2023 American Chemical Society)

The second aspect of the thesis focused on the evaluation of semi-empirical methods, which are less costly in terms of computing resources than pure DFT. Among these methods, GFN-xTB[3] has proved to be particularly promising, as it leads to much shorter computation times, with only a slight loss in terms of result precision. In particular, this method can be used to model electrolyte degradation reactions, the insertion of lithium ions between the graphene layers of the anode, the growth of Li salt nanoparticles (Li_2CO_3, LiF, Li2O) and the interaction between various organic electrolyte components and these inorganic nanoparticles [4].

Finally, research was started on two further aspects: the porosity of the SEI's porous organic layer and the diffusion of the electrolyte's main solvent[4] in this layer. The ongoing research should enable better estimation of the parameters used in phenomenological models, applied both in the automotive industry and at IFPEN for a better description of lithium battery aging.

[1-] Density functional theory is a method based on quantum physics that enables structures composed of several atoms to be studied and their physical-chemical properties including their chemical reactivity to be deduced.
[2-] Method used to simulate the behavior of systems evolving as a function of a master equation, using kinetic data related to elementary chemical reactions.
[3-] The GFN-xTB (Geometries, Frequencies, and Noncovalent interactions extended Tight-Binding) method is a semi-empirical quantum-mechanical approach for efficiently simulating molecular structures, reaction pathways and non-covalent interactions.
[4-] Ethylene carbonate.

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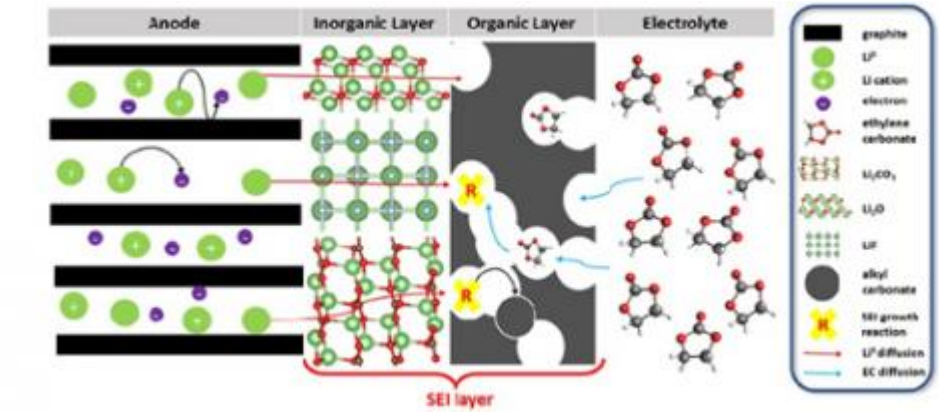

SC6 - How to better control loss of lithium battery capacity

Everybody knows that lithium-ion batteries, used in cell phones, computers, etc., gradually lose capacity and eventually fail. This loss of capacity is primarily due to a layer known as the SEI, which forms between one of the battery's electrodes and the electrolyte (see Figure). This layer already appears after the first battery charge/discharge cycle, and grows over time, consuming lithium ions. The process is irreversible and therefore detrimental to battery capacitye...

Batteries

Thermodynamics/Molecular modeling **Electrochemistry and corrosion**

Yves Chauvin Prize: Molecular modeling of the solid electrolyte interphase in lithium batteries

Thesis by **Daniel Carlos Da Silva**: « ***Développement d'une méthodologie de modélisation analytique des composants électriques dans un véhicule hybride : Optimisation des performances énergétiques*** »
(Development of a methodology for the analytical modeling of the electric components in a hybrid vehicle: energy performance optimization).

To maximize the contribution of hybrid electric vehicles (HEV) to the decarbonization of the transport sector, their energy performance is a key factor that needs to be considered from the design phase. For an HEV, optimizing the design in order to reduce consumption involves not only optimizing a sizing aspect but also the EMS[1]. This co-optimization of sizing and energy management is generally tackled either by nesting optimal control algorithms within an optimization algorithm dedicated to sizing, or by using convex optimization[2] to simultaneously optimize the design levels. However, the former approach is known to induce computational constraints (for example relating to calculation time), while the latter can affect modeling fidelity due to the constraints inherent in convex optimization.

Adopting a new perspective, this PhD research introduced a methodology for estimating powertrain energy consumption using a fully explicit formulation, illustrated in Figure 1. This was in the form of an EPCM[3], initially developed using component models, to consider power losses, and then predictive models, located at a second modeling level, in order to take into account the impact of component sizing variations.

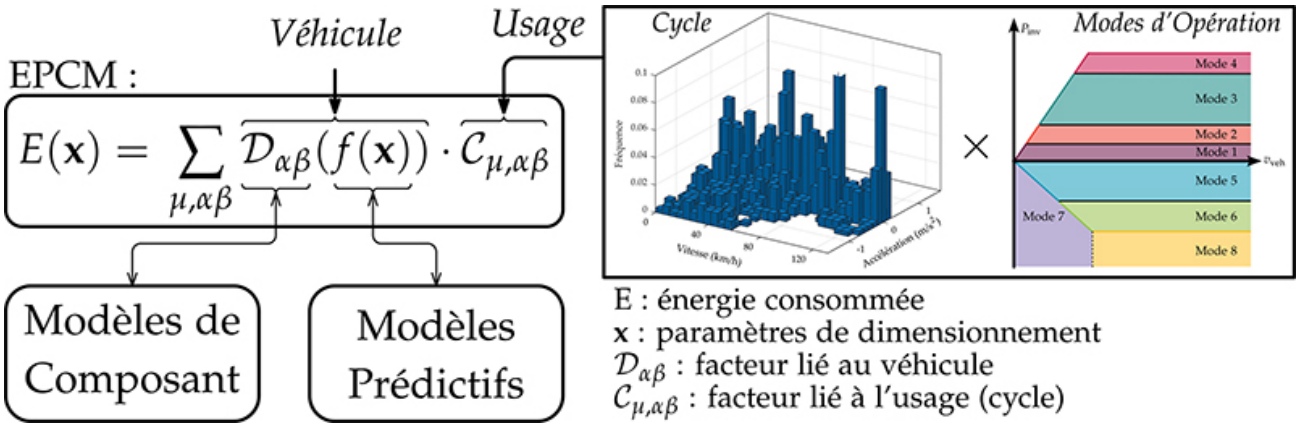

Figure 1: Structure of an Explicit Powertrain Consumption Model (EPCM)

The new methodology was developed using an FCHEV[4] as the reference. For vehicle energy analyses relating to the system as a whole, the research focused not only on modeling the components commonly found in electric vehicles, but also on modeling the power electronics and fuel cell system [1], aspects often neglected or inadequately addressed.

The *component models* were developed and validated using data obtained from a Toyota Mirai II during tests on IFPEN's roller test benches. Analysis of hydrogen consumption over test cycles

demonstrated a global error between measurement and model of less than 5 percent [2]. Operating data sets for components of various sizes were then used to develop *predictive models* based on regression analyses. Compared with the traditional use of performance maps, which are highly specific to each component, more general models like this introduced an error of less than three percent on hydrogen consumption. [3].

By exploring the use of the EPCM developed for the FCHEV, instead of an optimal control law, this thesis demonstrated that the use of an EMS employing a simple affine function provides a reasonable approximation for co-optimization in the early stages of vehicle design.

A computational performance analysis then showed that using the EPCM in a sizing optimization problem can reduce evaluation time by a factor of 200, while retaining both the sizing obtained with conventional modeling and an optimal EMS (Figure 2.a). This new formulation was also studied on reduced sizing problems[5], allowing us to obtain linear and quadratic expressions to approximate the hydrogen consumption obtained with a conventional formulation (Figure 2.b).

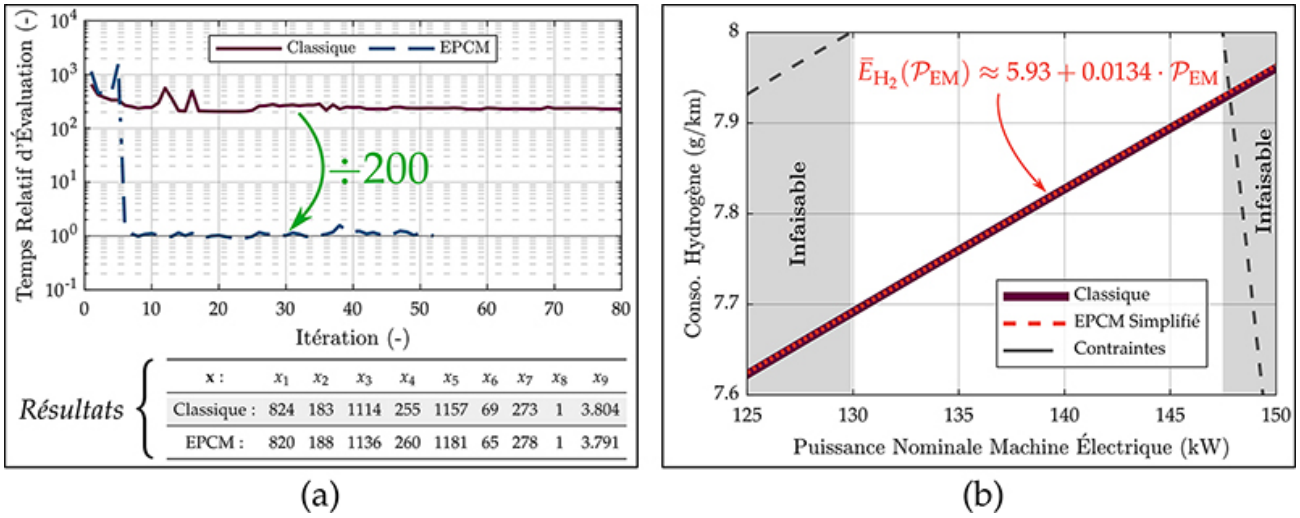

Figure 2:
?? (a) Comparison of evaluation time and optimization results using a conventional formulation and the EPCM.
(b) Comparison of the estimation of hydrogen consumption obtained using a conventional formulation and a simplified EPCM.

Once developed, such simple models can be used to draw rapid conclusions about the energy performance of an electric vehicle, and can be coupled with other key aspects of vehicle design, such as cost and life-cycle analysis.

1- Energy Management Strategy.
2- Where the objective function is convex (https://fr.wikipedia.org/wiki/fonction_convexe), as well as the feasible set (https://fr.wikipedia.org/wiki/Ensemble_convexe), which significantly facilitates optimization.
3- Explicit Powertrain Consumption Model.
4- Fuel Cell Hybrid Electric Vehicle.
5- i.e., with a reduced number of sizing variables, e.g., one or two.

6- i.e., using a quasi-static model for each component, with an optimal control law.

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Towards more explicit energy consumption for more efficient electric vehicles

Thesis by **Valentine Combaudon** : « ***Mécanismes et quantification de la génération d'hydrogène naturel en contexte intracratonique : le cas du Mid-Rift System (Kansas, USA)*** » **(Natural hydrogen generation mechanisms and quantification in an intracratonic context: the Midcontinent Rift System (Kansas, USA).**

For the last ten years or so, geologists have been fascinated by the natural hydrogen (H_2) emitted within "cratons", in the heart of continents. While its presence in subsurface has been identified in many places around the globe, it remains to be ascertained whether the use of this decarbonized energy source is likely to be economically viable. To answer this question and then identify the drilling sites with the greatest potential, large-scale quantification of this resource requires the use of modelling.

Moreover, while the origin and quantity of H_2 emitted from the seafloor has been largely understood for decades, the potential of the various minerals in cratonic rocks to produce it, via water-rock interaction reactions, remains unknown. Questions about the source of H_2 is nonetheless essential in order to assess the corresponding resource.

This PhD research set about examining the issue, taking as its subject the North American Midcontinent Rift System (MRS) composed of ancient rocks (over 1 billion years old) and extending over thousands of kilometers. The study of these rocks was based on a multi-scale approach (from nm to cm) for which an analytical workflow was developed (Figure 1), based on different observation techniques: microscopy for phase identification, synchrotron for chemical speciation and µ-tomography for estimating volumes of altered minerals [1]. The application of these imaging techniques to various rocks in the Kansas basement, south of the rift, has made it possible to quantify the potential of the geological formations in place to produce natural hydrogen by quantifying the reduced iron in minerals, as well as to estimate the resources already produced via the quantification of oxidized iron.

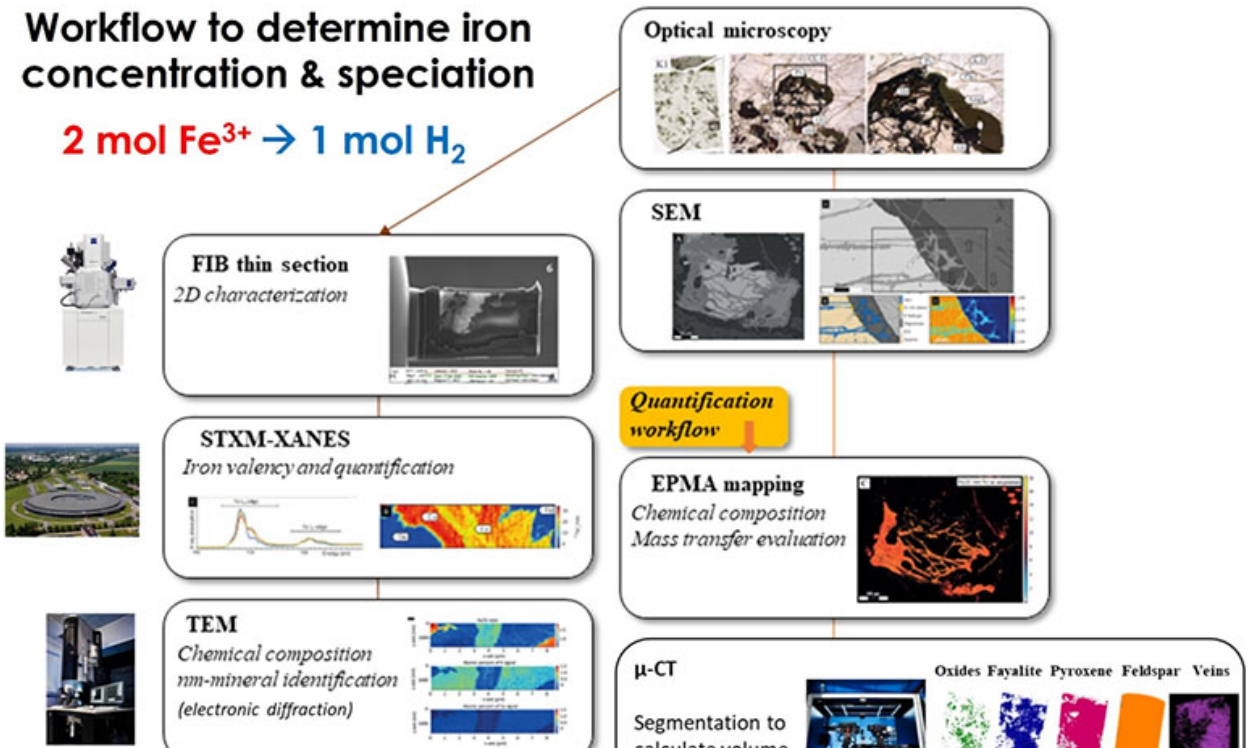

Figure 1: Analytical workflow used to quantify H2 potential from a multi-scale rock study.

The implementation of this workflow has enabled the identification of the H_2 source rock and the complete characterization of the “hydrogen system” in the southern part of the rift [2] (Figure 2). In addition to this source rock (or generating rock), the reservoir rock and then the cap rock are found above, and it appears that the production of this decarbonized resource remains active there, even though the rocks in question are far older than the oil reservoirs, where fossil hydrocarbons are produced.

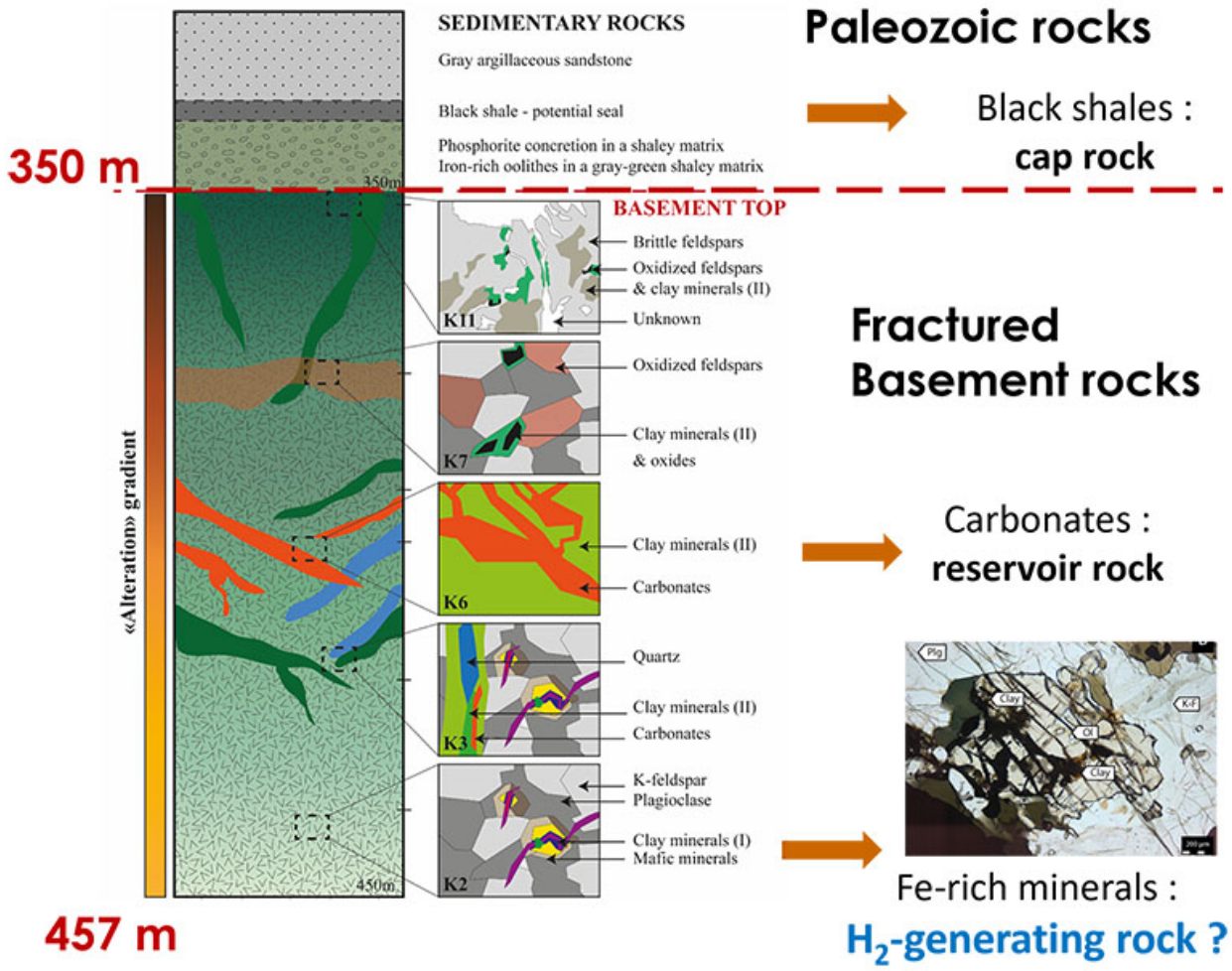

Figure 2: Characterization of the Hydrogen system in the southern part of the rift, in the Kansas Precambrian basement.

Finally, the same characterization was conducted for the northern part of the rift, in Minnesota where active surface hydrogen production occurs at the outcrop of Precambrian rocks. This characterization made it possible to identify new H_2 production and consumption markers, in the form of volatile fatty acids, in hyper-basic and highly chemically reduced waters [3]. Such compounds result from the biological consumption of H_2, or from its chemical reactivity with inorganic carbon such as CO_2.

The knowledge acquired during this research, as well as the analysis protocols developed, have been integrated into IFPEN’s commercial solutions aimed at identifying and characterizing exploration

zones. The protocols are now being used to study other emitting sites, with the aim of producing numerical models for predicting potential subsurface resources in the very near future.

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“Continental” natural hydrogen: better understand in order to better harness its potential

Thesis by **Yuna Han**: « ***Optimisation de la porosité et de l'acidité de zéolithes large pore pour la transformation de sucre en molécules plateforme*** » **(Optimization of large-pore zeolite porosity and acidity for the conversion of sugars into platform molecules).**

Biomass conversion into chemical products and intermediates is increasingly being adopted to reduce the carbon footprint of the industry concerned. Among biomass-based resources, sugars are extremely attractive since they contain a lot of functional groups enabling their conversion to products of interest (alcohols, acids, etc.). For example, through fructose dehydration, it is possible to obtain 5-hydroxymethylfurfural (5-HMF), a molecule that can be used to produce polymers. Since the conversion of fructose to 5-HMF is catalyzed by Brønsted acids[1], liquid acid catalysts in solution are currently used, but without the possibility of recycling this catalyst. The development of a solid acid catalyst is thus crucially important.

Zeolites are porous materials that appear to be particularly interesting for this application, firstly because they are strong Brønsted acids, and secondly because their restricted pore space can limit the formation of undesirable oligo- or polymerized co-products. However, sugars are fairly bulky molecules and their diffusion in a zeolite's micropores is slow, even for so-called "large-pore" zeolites such as faujasite. Accelerating this diffusion in the case of fructose would thus make it possible to increase catalytic activity for its conversion, and the production of a hierarchical porosity system, facilitating access to the micropores, is a way of achieving this. Such was the subject of this thesis.

In this thesis, treatments in basic media were used to generate a mesoporous porosity scale in USY-type (Ultra Stable Y zeolite) faujasite zeolites. Basic treatment selectively dissolves the silicon in the zeolite structure, without affecting the aluminum that generates the Brønsted acidity: this is known as desilication. It was necessary to find a compromise between mesopore generation and the destruction of the zeolite's crystalline structure. These zeolites were then tested for the conversion of fructose into 5-HMF in order to evaluate the effect of the mesoporous system generated on catalyst activity and selectivity.

Initial work demonstrated how the addition of tetra-alkylammonium ions, with different alkyl chain lengths, during basic treatment, can regulate the degree of desilication and, therefore, mesopore formation. [1]. In this respect, the aluminum content of the parent zeolite also plays a very important role. (Figure 1).

The effect of mesopore generation on Brønsted acid site accessibility was then measured by adsorption of a basic molecule with a high steric hindrance, making it possible to define rules for the purposes of optimizing this property. While it intrinsically increases the rate of 5-HMF production from zeolite catalysts, the concentration of accessible acid sites does not, in itself, make it possible to explain the benefit of zeolites in fructose conversion. A chemometric analysis was carried out to look for other explanatory factors. In particular, the analysis identified low residual Lewis acidity[2] and a low Al concentration in the catalyst, the latter possibly indicative of the hydrophobicity of the zeolite, as decisive criteria.

Another component of the research consisted in looking for fructose conversion reaction pathways. Analytical and spectroscopic techniques showed that 5-HMF is not a “primary” product, but that the reaction passes through dehydration intermediates of the cyclic form of fructose [2], providing a new insight into a debate hitherto unresolved in the literature.

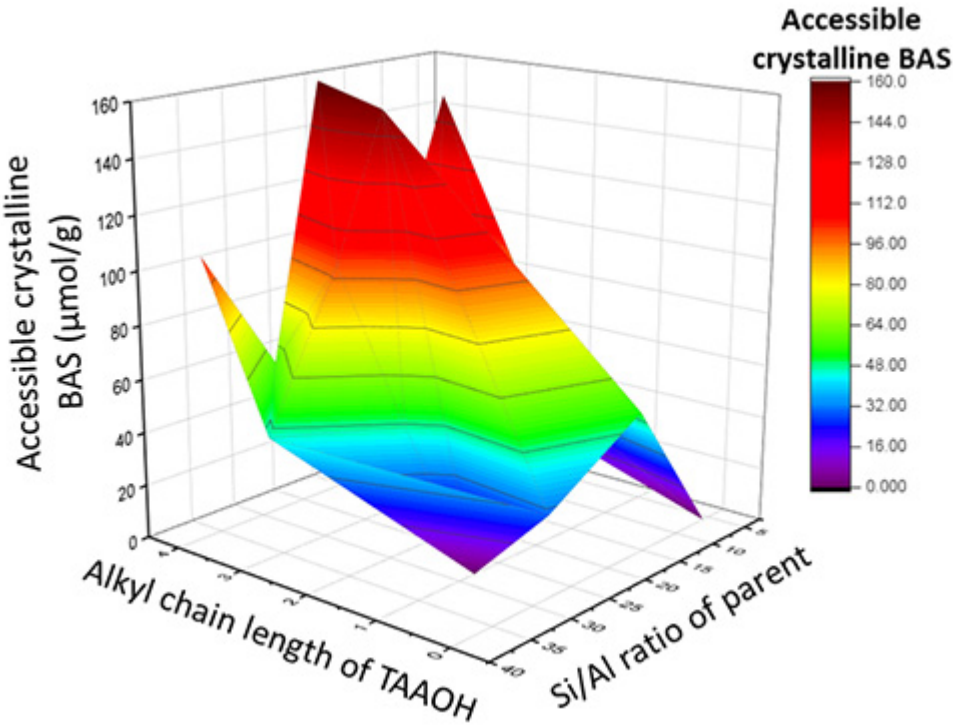

Figure 1: Concentration of accessible acid sites as a function of the tetra-alkylammonium cation and the Si/Al ration of the parent USY zeolite.

This research has considerably advanced our knowledge of zeolite acid site porosity and accessibility modification. It has also provided a better understanding of the mechanisms involved in sugar conversion by zeolites. Nevertheless, some questions remain unanswered, such as a potentially important role of zeolite hydrophobicity in sugar conversion. This point has led to IFPEN initiating a new research program aimed at gaining a better understanding of the adsorption of water (a by-product of dehydration) in USYs with hierarchical porosity.

1- “Proton donor”-type acid.
2- A Lewis acid is a chemical species that can accept an electron pair and thus create a covalent bond.

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How to prepare better zeolite catalysts for the conversion of sugar

Thesis by **Antoine Sabrié** : « ***Proposition et mise en œuvre d'une topologie d'onduleur multifonctionnel à tension de bus régulée pour la traction électrique*** » **(Proposal and implementation of a multifunctional inverter topology with regulated bus voltage for electric traction).**

In electric vehicle powertrains, it is necessary to convert the DC voltage supplied by the battery into three-phase AC voltages to power the vehicle's electric motor. This conversion is carried out by the vehicle's on-board power electronics, known as an inverter. This inverter is also responsible for controlling the electric motor, varying its speed or torque.

Ideally, we would like to be able to convert all of the available voltage to drive the electric motor. In reality, due to the principle inherent in inverter conversion, the motor can only be supplied with AC voltages whose maximum amplitude is 57% of the voltage value delivered by the battery. In addition to this limitation, associated with the structure of the topology used, variable voltage drops may occur in the powertrain. These can occur, for example, as a function of the battery's state of charge, or as a function of the temperature at which powertrain components operate. These voltage drops, be they intrinsic or of external origin, will reduce the performance of the machine in question.

Initially, this PhD research made it possible to study and model in detail the physical phenomena behind intrinsic voltage drops in converters. To this end, an analytical model was proposed and compared with experimental data, demonstrating a good estimation of these phenomena [1].

In industry, a solution used to overcome inverter voltage limitation is to add a DC-DC step-up converter interfaced upstream the inverter. The drawback with this solution is that it introduces a second conversion stage that can impact the powertrain's global performance and reliability. Moreover, in recent years, new architectures have been considered to pool conversion functions and thus reduce the cost, volume and weight of the powertrain while improving its overall efficiency. As a result, single conversion stage step-up inverter architectures, without the addition of a supplementary DC-DC conversion stage, have been proposed in the literature. One of these recently emerged architectures, the SSI[1], offers competitive advantages over its counterparts. Nevertheless, we demonstrated that this converter was incompatible with the electric powertrain [2]. The latter loses a degree of freedom needed to drive an electric motor, and lacks the capacity to recover energy during braking, a function that is also essential for traction applications.

To overcome these limitations, we introduced a new inverter: the B-ASSI [2]. Compatible with traction applications, it was designed and experimentally validated with a proof of concept of a few kW (Figure 1(a)). A new Pulse Width Modulation and an appropriate control law for the converter were also developed. The results show that B-ASSI offers access to more operating points and better efficiency than traditional converters (Figure 1(b)).

Finally, this research has paved the way for the addition of an inverter supply voltage step-down function, which optimizes low-speed operation, reducing inverter temperature and torque oscillations and ultimately improving the performance of the electric motor [3]. A B-ASSI extension, incorporating this functionality has been proposed and experimentally validated.

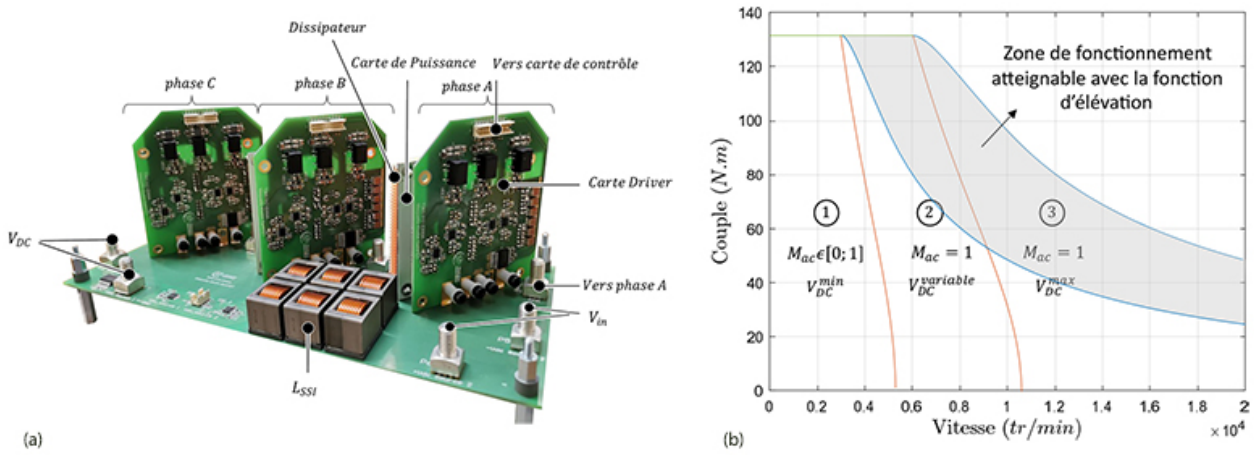

Figure 1: (a) Proof of concept of the B-ASSI developed in this PhD research.
(b) Extension of the electric motor's theoretical operating zone using the B-ASSI compared to a conventional inverter.

This research paves the way for a wider application of Split Source architectures in electric traction, while highlighting the advantages of combining several functions in a single converter to optimize the powertrain.

[1-] Split Source Inverter.

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Towards a new generation of power converters to optimize electric powertrains

Thesis by **Omar Maiga**: « ***Caractérisation géologique et géophysique 3D d'un système de réservoirs d'hydrogène naturel - Exemple du champ de Bourakèbougou, Mali*** » **(3D geological and geophysical characterization of a system of natural hydrogen reservoirs - Case of the Bourakebougou field, Mali).**

In the current drive to find ways to produce inexpensive, green hydrogen, the natural hydrogen found underground is attracting growing interest as a component of a new energy mix.

In Mali, the Bourakebougou field is the emblematic benchmark for natural underground hydrogen accumulations of this type today: 25 exploratory boreholes have demonstrated its presence in high concentrations (98 mol%), both in a geological reservoir located around one hundred meters below the surface and in other reservoirs at greater depths.

In order to better characterize these reservoirs and the hydrogen retention and preservation processes at play, PhD research was conducted at IFPEN, in partnership with the field operator Hydroma.

An in-depth study of coring and logging[1] results, as well as of the geochemical data obtained, was carried out in order to better characterize the nature of Bourakebougou's hydrogen reservoirs [1].

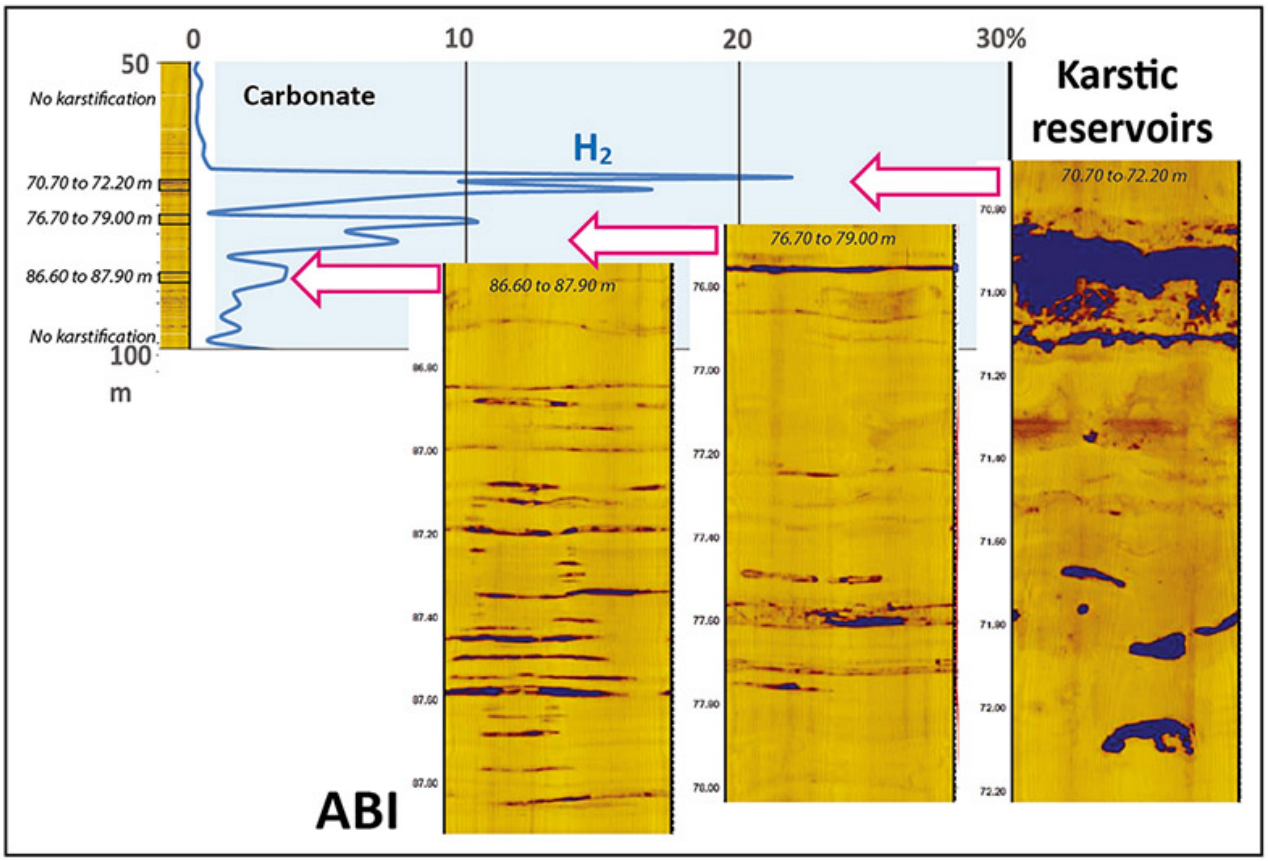

Figure 1: Drilling acoustic imaging in the main reservoir (karstified carbonates) containing Hydrogen (98 mol%) at the Bourakebougou field compared with gas logging results. From [1]

The main reservoir - the shallowest and with the highest concentration - is made up of dolomite carbonates (cap carbonates from the late Proterozoic glacial period). The majority of these carbonates are karstified[2] and present a high degree of heterogeneity in terms of porosity (0.21-14.32%). Based on analysis of borehole imaging data from carbonate reservoirs (the shallowest main reservoir and other deeper secondary reservoirs), hydrogen accumulation primarily occurs in karstic cavities (Figure 1). Other reservoirs, particularly the deeper ones, are made up of porous sandstone rocks with much more homogeneous porosities (4.52-6.37%) than massive carbonates.

By comparing the reservoir system studied with classic oil and gas systems, it can be observed that the hydrogen reservoir is a dynamic system that gradually becomes recharged with hydrogen-rich gas at a rate similar to that of extraction. This can be explained by the fact that hydrogen, most of which is dissolved at depth in deep aquifers (as confirmed by logging data), is released as a result of the drop in pressure associated with production. It therefore recharges the upper karstic reservoir in the form of a gaseous phase, enabling a relatively constant pressure to be maintained on the scale of a few years.

The significant mobility of hydrogen molecules, due to their very small size, gives them highly diffusive properties leading to the frequent surface seeps recently recorded all over the world. It is for this reason that most of the discussions surrounding natural hydrogen exploration focus on its surface occurrences and the processes involved in its production. However, the hydrogen trapping capacity and process are the most critical issues in attempting to discover gas-phase accumulations that are both significant and conducive to profitable production. It is for this reason that in a different phase of this PhD research, a detailed characterization of cap rocks (in this case dolerite rocks) containing hydrogen in the Bourakebougou field was conducted [2].

This study revealed that the sealing capacity of dolerites is linked to the fact that they are only slightly fractured and none of the fractures are open. The role of aquifers was also highlighted as contributing to subsurface hydrogen retention. As the latter is not very soluble in water, in low pressure and temperature conditions, it becomes less and less likely to diffuse easily to the surface from the shallow depth of the main reservoir.

In conclusion, this study underlines the fact that the exploration of natural hydrogen fields should not be based only on the presence of a generation process, but also on the presence of a highly efficient trapping system.

[1-] Continuous physical recording of variations, as a function of depth, of a given characteristic of formations encountered during a survey.
[2-] A karst is a geomorphological structure resulting from the hydrochemical and hydraulic erosion of all soluble rocks.

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>> https://doi.org/10.1016/j.ijhydene.2023.10.131

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Natural hydrogen: subsurface accumulation process - Example of the Bourakebougou H2 field in Mali

Thesis by **Thomas Pigeon**: « ***Méthodes d'échantillonnage d'évènements rares et machine learning pour l'étude des mécanismes de réaction catalytiques*** » **(Rare event sampling methods and machine learning for the study of catalytic reaction mechanisms).**

Understanding the chemical properties of the supports (alumina-gamma in particular) and active phases of heterogeneous catalysts is a challenge that requires a detailed atomic scale description of systems and the quantification of events that are rare on this scale: chemical reactions.

Quantum simulation appears to be a suitable tool for trying to overcome this challenge. However, continuous improvement of numerical methodologies and atomistic models is required to determine the complex structure of active sites, on the one hand, and their reactivity (rate constant), on the other. By covering all these aspects, this PhD research has provided answers to this dual challenge, while exploring the contributions of machine learning (ML) to the understanding of the active sites.

Transition State Theory (TST) inevitably overestimates reactivity. The latter is very often coupled with a harmonic approximation of the potential energy surface (hTST), implying a second source of uncertainty related to the rate constant calculation. To overcome these difficulties, an alternative approach was implemented to calculate reaction rate constants directly. This approach combines a rare-event simulation method AMS[1] with AIMD[2], implemented with quantum software (such as VASP[3]) widely used by the community (Figure 1a).

First of all, ML tools (SVM [1], Autoencoders [2]) made it possible to identify the collective variables (CVs) used to automatically define the progress of AMS during a reaction (Figure 1b). They were also used to build an interatomic force field that accelerated AIMD calculations. Using SVM, AMS and AIMD, the rate constants of rotation and dissociation of a water molecule on the surface (100) of alumina-gamma[1] were evaluated. These constants turn out to be up to two orders of magnitude lower than those obtained with the hTST approach, revealing the errors generated by the latter [1].

In parallel, with a view to a more detailed description of the active sites present on alumina-gamma crystallites, several complex facet [3] and edge [4] models were developed. These were used to provide a more detailed interpretation of the proton's experimental NMR[4] spectra (Figure 1c). Ab initio calculations led to the identification of previously undocumented sites located on edges.

This research, conducted within the dual context of the INRIA-IFPEN framework agreement and the ENSL-IFPEN ROAD4CAT chair, is now being continued as part of the MAMABIO project, attached to PEPR B-BEST.

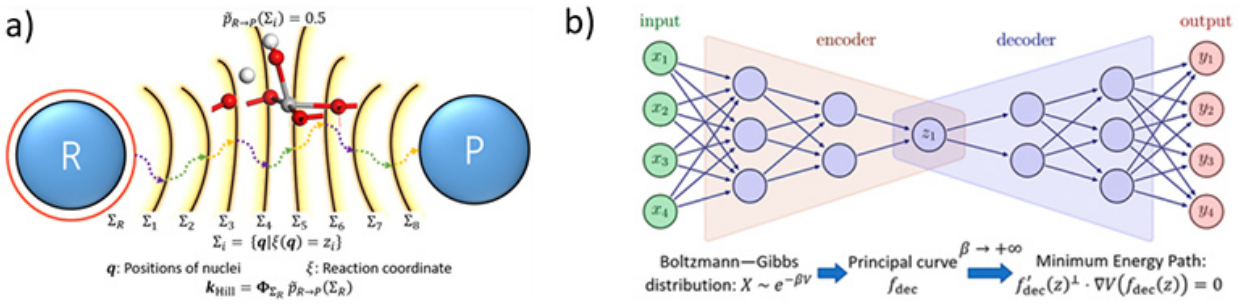

Figure 1:
a) Diagram of the estimator constructed by AMS to estimate rate constants,
b) Illustration of an auto-encoder and the physical meaning of the CVs learned by this method,
c) Assignment, based on atomistic models, of 2D 1H NMR signals to hydroxyls of surface and edge sites of gamma alumina.

1- Adaptive Multilevel Splitting
2- Ab Initio Molecular Dynamics
3- Vienna Ab-initio Simulation Package, https://www.vasp.at/
4- Nuclear Magnetic Resonance

References:

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Advanced reaction rate constant calculation methodologies for innovative catalyst models

Thesis by **Théo Martinez**: « ***Impact des paramètres hydroclimatiques et anthropiques sur la dynamique sédimentaire du système deltaïque du Rhône à la transition Holocène-Anthropocène*** » **(Impact of hydroclimatic and anthropogenic parameters on sedimentary dynamics of the Rhône delta system at the Holocene-Anthropocene transition).**

Coastal systems such as deltas are vulnerable to sea-level rise and erosion. The stability of deltas depends on the sedimentary input produced in the watershed, which is strongly impacted by climatic and anthropogenic factors, whose variations and increasing pressure lead to problems of resource management (aquifers) and land-use planning (bank instability, flood management, etc.).

In order to predict the impact of different environmental change scenarios and thus enable the implementation of appropriate local policies, it is essential to have modeling tools capable of integrating the various hydroclimatic and anthropogenic parameters and their temporal evolution. The development of numerical models capable of describing the factors modifying the natural environment is therefore necessary. Such models need to be parameterized, and the main challenge is to quantify the different forcing parameters[1] and their consequences on the environment at different timescales.

The evolution of the Rhône delta since the last Quaternary glaciation is the ideal laboratory for studying human-environment interactions and their impact on the environment. The chronostratigraphic evolution[2] of the Rhône delta and the river corridors of the upstream Rhône is well documented. Digital interpretation of old maps and satellite data has also enabled us to trace the evolution of land use over the last three centuries at watershed scale [1], which was then translated into erosion potential and flows of particles transported to the delta.

Using the stratigraphic model DionisosFlow^{TM} software, these data were used to calibrate a stratigraphic model of the delta's past evolution and to reconstruct six main Holocene[3] hydrosedimentary flow phases, with a marked threshold from 3000 cal. BP[4] onwards.

On this basis, predictive scenarios for the evolution of the deltaic system were proposed (Figure 1) [2].

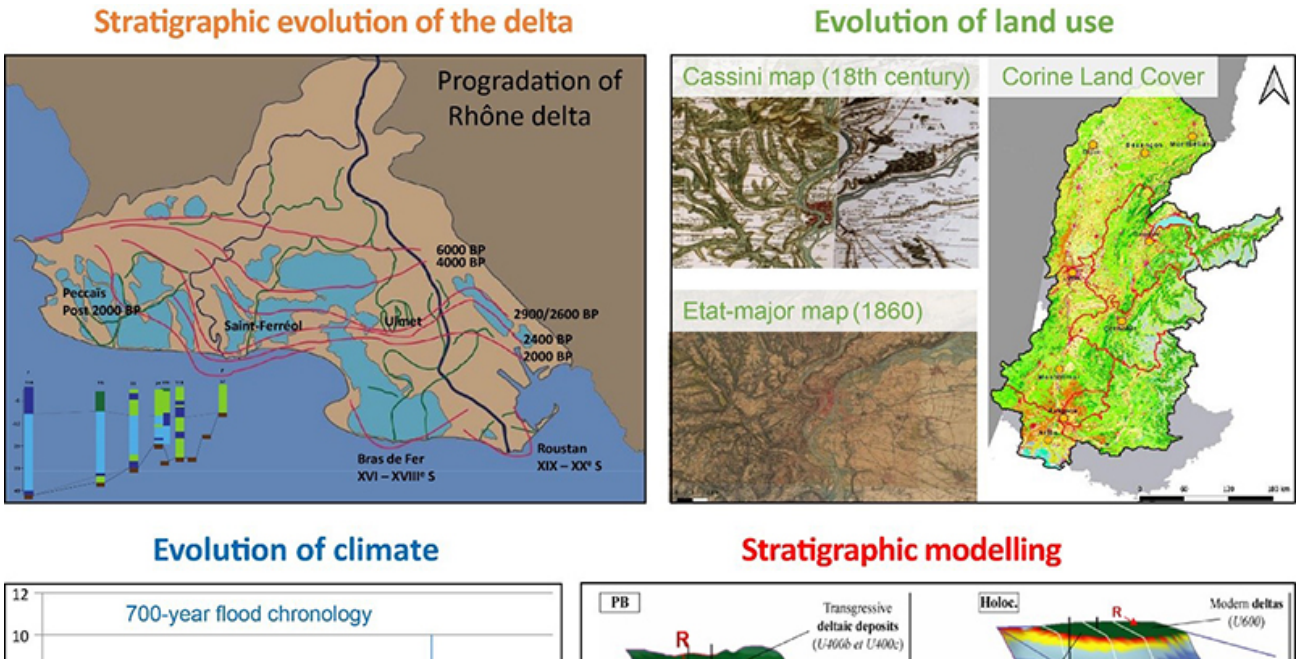

Figure 1: Integration strategy of
1- sedimentary analysis of the delta,
2- Estimation of volumes of sediments eroded in the catchment area from analysis of ancient maps,
3- Holocene climate evolution, in order to
4- calibrate a stratigraphic modeling approach.

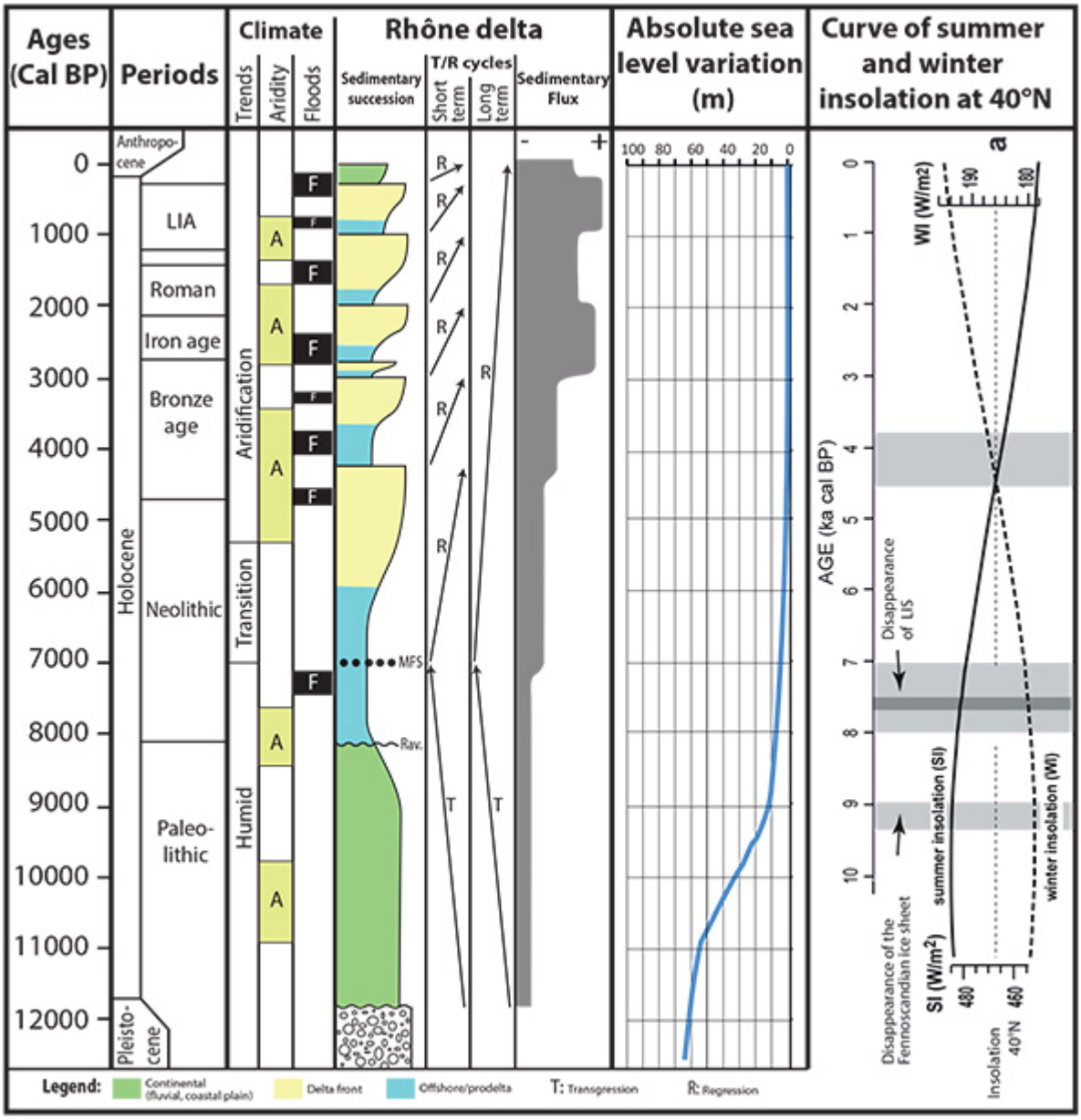

Figure 2: Stratigraphic evolution of the Rhône delta and sedimentary flows over Holocene period in relation to changes in sea level and climatic.

The volume of sediments associated with the different phases of the Rhône delta construction over the last 11,700 years were calculated through a high-resolution stratigraphic study:

- It took more than 4,000 years for the Rhône delta to start to develop around the year 7,000 cal. BP. The estimated sedimentary volumes from the mid-Holocene period to the late Holocene period are associated with hydroclimatic events.

- Changes in sedimentation rates, associated with periods of climatic and anthropogenic forcing phenomena, are identified around 3,000 cal. BP.

These changes appear to represent a major bifurcation with more extensive and intensive human forcing from this period (Figure 2) [2].

The results of prospective simulations indicate that in the absence of an increase in sedimentary flow, the delta coastline could retreat by several kilometers by the year 3,000, with a 60% reduction in its surface area (Figure 3). To compensate for a 50 cm/century rise in sea level (optimistic scenario), sedimentary flow would have to be three times greater than the present-day flow, and five times greater for a 90 cm/century rise (pessimistic scenario).

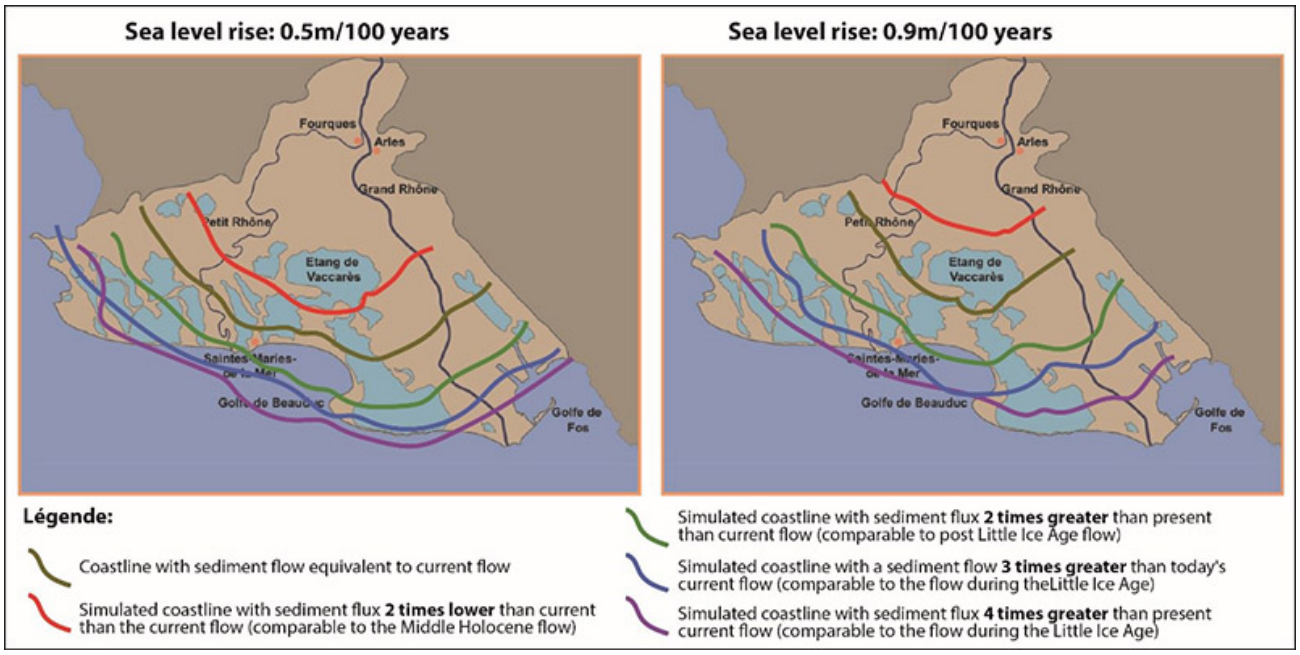

Figure 3: Evolution of the Rhône delta coastline to the year 3,000 obtained
by modeling two rising sea level scenarios:
0.5 m/100 years (optimistic IPCC scenario)
and 0.9 m/100 years (pessimistic IPCC scenario).

On the basis of quantitative data relating to hydrosedimentary flows reproduced for the past 12,000 years, this research provides an insight into the future evolution of a delta system such as the Rhône. Thus, in addition to the methodology developped in this thesis work, it illustrates the ability of numerical simulations to produce predictive scenarios of coastal evolution associated with anthropogenic or climatic activity.

1- i.e., the external constraints applied to a system in equilibrium.
2- Relative to the organization and division of rock strata as a function of their age relationships.

[3-] Geological period extending over the last 12,000 years.
[4-] Calendar years before the present.

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Impact of hydroclimatic and anthropogenic parameters on past and future Rhône delta dynamic

Thesis by **Mathis Pasquier** : « ***Quantification d'incertitudes pour la dispersion turbulente de polluants à l'échelle micro-urbaine*** » **(Uncertainty quantification for the turbulent dispersion of traffic-related pollutants on a micro-urban scale).**

In urban zones, road traffic is responsible for a high proportion of pollutant emissions, with a significant impact on air quality, which represents a major public health issue. Atmospheric dispersion can be comprehensively taken into account using CFD[1]. However, random uncertainties, of both natural and anthropogenic origin, can affect its predictive capacity.

Concerning this prediction, the PhD research was aimed at quantitatively evaluating the impact of uncertain parameters: firstly, meteorological and, secondly, those related to road traffic. To do this, "high-fidelity"[2] simulations of pollution dispersion on a micro-urban scale (neighborhood) were conducted.

Initially, a complete modeling chain was constructed in order to produce two-dimensional spatial representations of pollutant concentrations in real urban geometries. This combined a CFD code based on the Lattice Boltzmann method (LBM), a microscopic traffic simulator (vehicle scale) and a road traffic emissions model. This LBM code was developed for highly turbulent flows and validated on academic test cases before being applied to realistic road geometry and emissions, in this case NOx emissions (Figure 1).

The subsequent calculations demonstrated that consideration of non-uniform emissions data, associated with the acceleration/deceleration phases of vehicles using urban roads, modified the estimation of inhabitant pollution exposure [1].

A sensitivity analysis was then conducted using this calculation chain, in order to identify which input uncertainty sources have the greatest impact on outputs of interest. To this end, substitution models[3], which are inexpensive to evaluate, were constructed, in order to reduce CFD simulation time.

The outputs examined were time-averaged maps related to pollutant concentration and to the probability of threshold exceedance. The uncertainty input variables were: wind direction and speed, traffic volume and composition (proportion of diesel and gasoline vehicles), as well as the road network speed limit. In this way, 2D spatial sensitivity maps (Figure 2) and global sensitivity indices for the entire domain were obtained [2].

Conducted on a local scale and with data reflecting the most realistic conditions possible (geometry, weather, emissions), this study concluded that wind direction and the proportion of diesel engines were the most influential factors.

The research also highlighted the interest of the type of approach employed, combining CFD with statistical methods, to understand the influence of multiple parameters in complex scenarios. In terms of application, this makes it possible to objectively assess the impact of a given planning or regulatory decision.

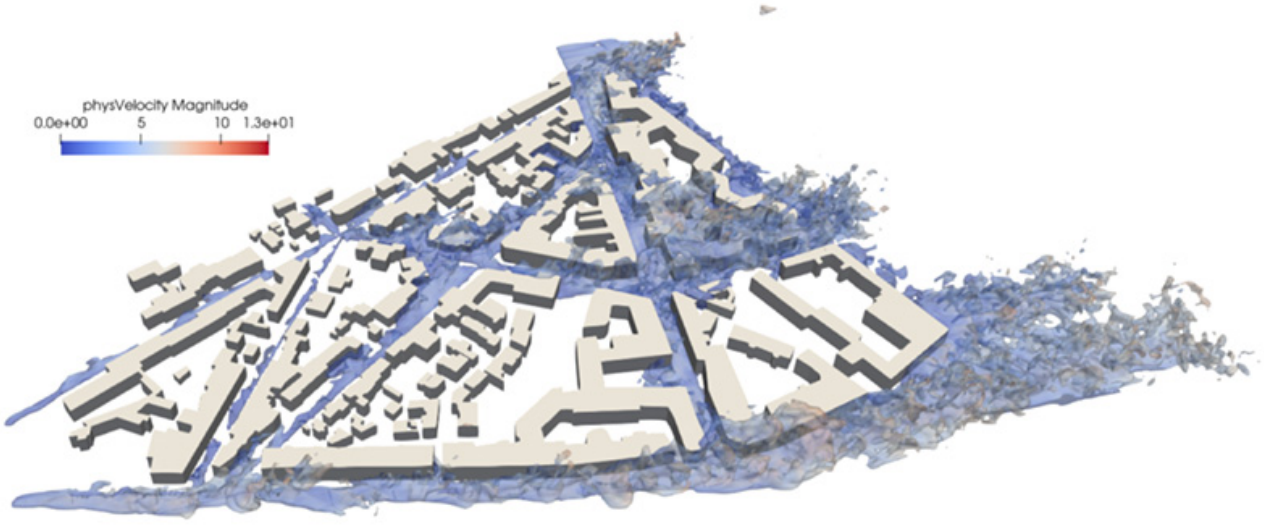

Figure 1: iso-contours of pollutant concentrations under a westerly wind in an urban neighborhood in the Paris suburbs with non-uniform stationary emissions from road traffic.

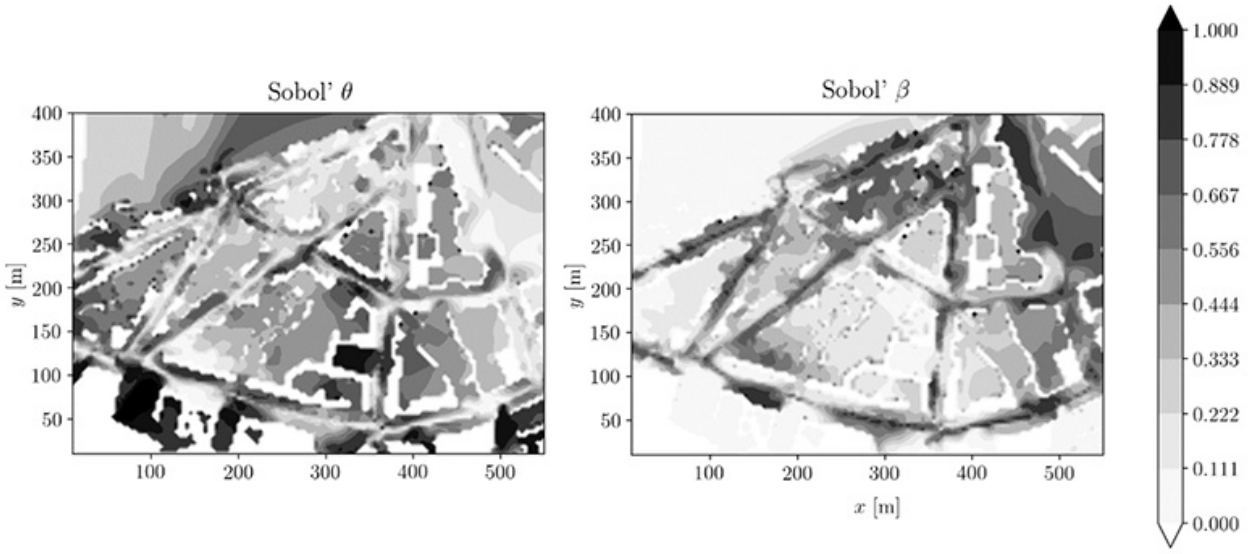

Figure 2: 2D maps of Sobol' indices (4) demonstrating the relative contribution of incoming wind angle (left) and the proportion of diesel/gasoline engines (right).
et de la proportion de moteurs diesel/essence (à droite).

1- Computational Fluid Dynamics.
2- Enabling consideration of turbulence.
3- Proper Orthogonal Decomposition combined with Gaussian Processes Regression (POD-GPR).
4- Sensitivity index of an output variable with respect to an input variable (based on variance decomposition).

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Uncertainty quantification for the turbulent dispersion of traffic-related pollutants on a micro-urban scale

Thesis by **Joudy Dankar**: « ***Mechanistic study of the photocatalytic reduction of CO_2 over Pt/TiO_2 using an operando FTIR approach*** »

The photocatalytic reduction of CO_2 to "C_1/C_2 solar fuels"[1] is an attractive conversion reaction since it has the advantage of eliminating this greenhouse gas while providing a usable product .

However, despite extensive research efforts, the level of CO_2 conversion remains very low, even for the most active catalysts on the market, and the reaction mechanisms involved is still poorly understood.

In order to remedy this, this PhD research focused on the study of a model Pt/TiO_2-type photocatalytic system. For the purpose of the study, an operando methodology[2] was deployed combining several techniques:

- infrared spectroscopy (FTIR) to characterize the irradiated catalyst surface;
- mass spectrometry and gas phase chromatography to analyze the gaseous effluents generated.

This approach made it possible to determine correlations between the structure/surface of the catalyst and its activity. In addition, various "ex situ" analyses were carried out, including Thermogravimetric Analysis (TGA), X-ray Photoelectron Spectrometry (XPS), Transmission Electron Microscopy (TEM), as well as the processing of spectral data using a chemometric approach (MCR-ALS) and the use of isotopes in specific operando FTIR measurements ($^{13}CO_2$, D_2O). This made it possible to determine the factors governing the photocatalytic activity of the system studied.

The information obtained underline in particular: i) the importance of the presence of carbon impurities on the catalyst surface (leading to an overestimation of activity) [1] ii) the beneficial effect of cycled irradiation conditions [2] and iii) the central role of acetate species in the CO2 photoreduction reaction [3].

These observations reveal the complex dynamics involved in the photocatalytic reduction of CO_2. They also provide a potential lever for improving the performance of the photocatalyst for the reaction via modulation of the surface chemistry/properties and/or reaction conditions.

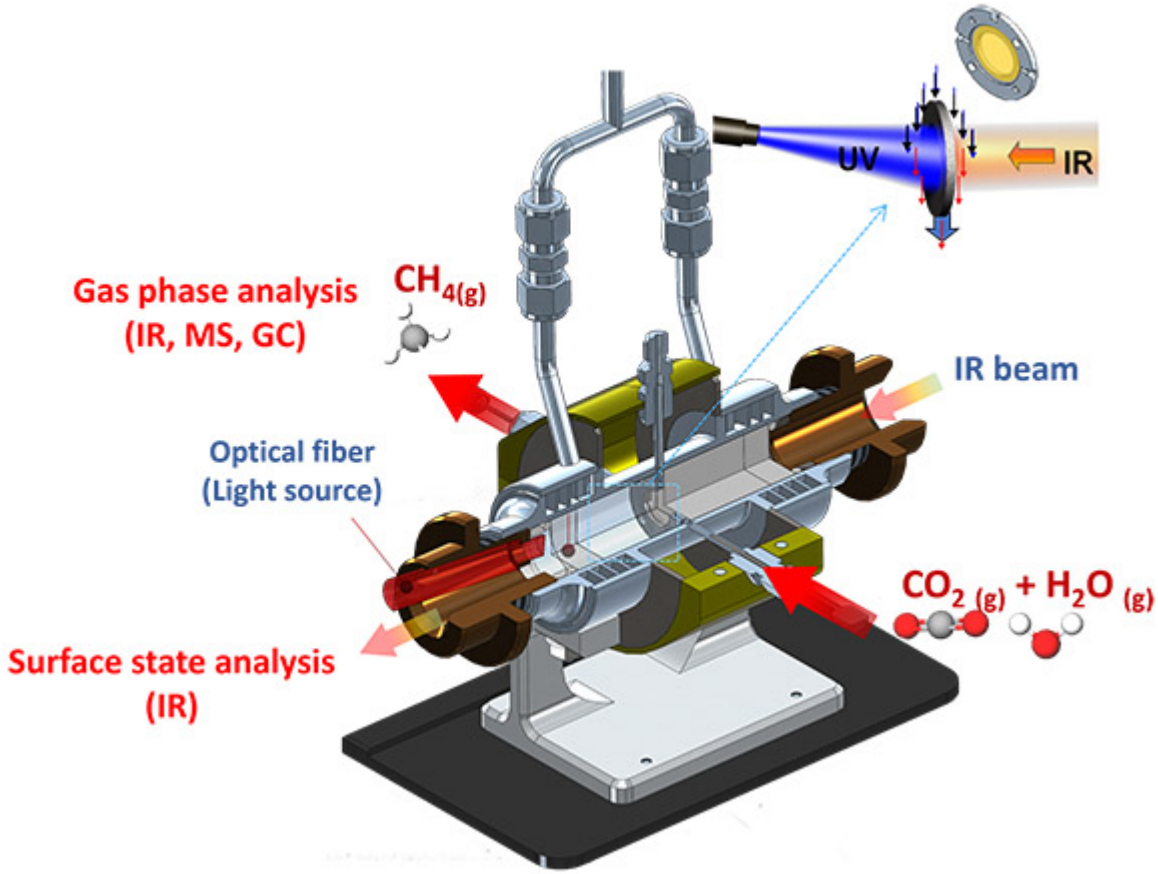

Figure 1: Diagram of the spectro-photoreactor for simultaneous analysis of the irradiated surface (IR) and outgoing effluents (IR, MS, GC).

1- Syngas, methane/methanol, formic acid, C2 + liquid fuels.
2- In reaction conditions, with monitoring of changes and products.

References:

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Elucidation by operando infrared spectroscopy of CO2 photoreduction mechanisms on Pt/TiO2 catalysts

Thesis by **Anne-Sophie Esneu**: « ***Étude des mécanismes d'endommagement des formations lors de la réinjection des fluides géothermiques*** » **(Study of formation damage mechanisms during geothermal fluid reinjection).**

Injectivity in geological formations is a well documented factor in fields related to new energies and the climate (geothermal energy, underground CO_2 storage, etc.). The clogging of geological formations, a recurrent problem causing injectivity losses, is associated with the fact that reinjected water frequently carries a high concentration of suspended organic and mineral elements, in the form of colloidal particles. To attempt to overcome this clogging, or at the very least minimize it, it is important to have a clear understanding of the mechanisms at work.

Such was the aim of this PhD research conducted using a microfluidics approach (Figure 1) combining two visualization techniques: optical imaging [1] and laser-induced fluorescence [2]. It made it possible to identify different deposition sites and regimes, as well as to describe clogging mechanisms, including the identification of a shear-induced aggregation phenomenon [3]. The body of results obtained using microfluidics was validated for more real systems (for example, a suspension of polystyrene particles in reconstituted sand beds or clay particles in micromodels) and paved the way for potential solutions to the phenomenon.

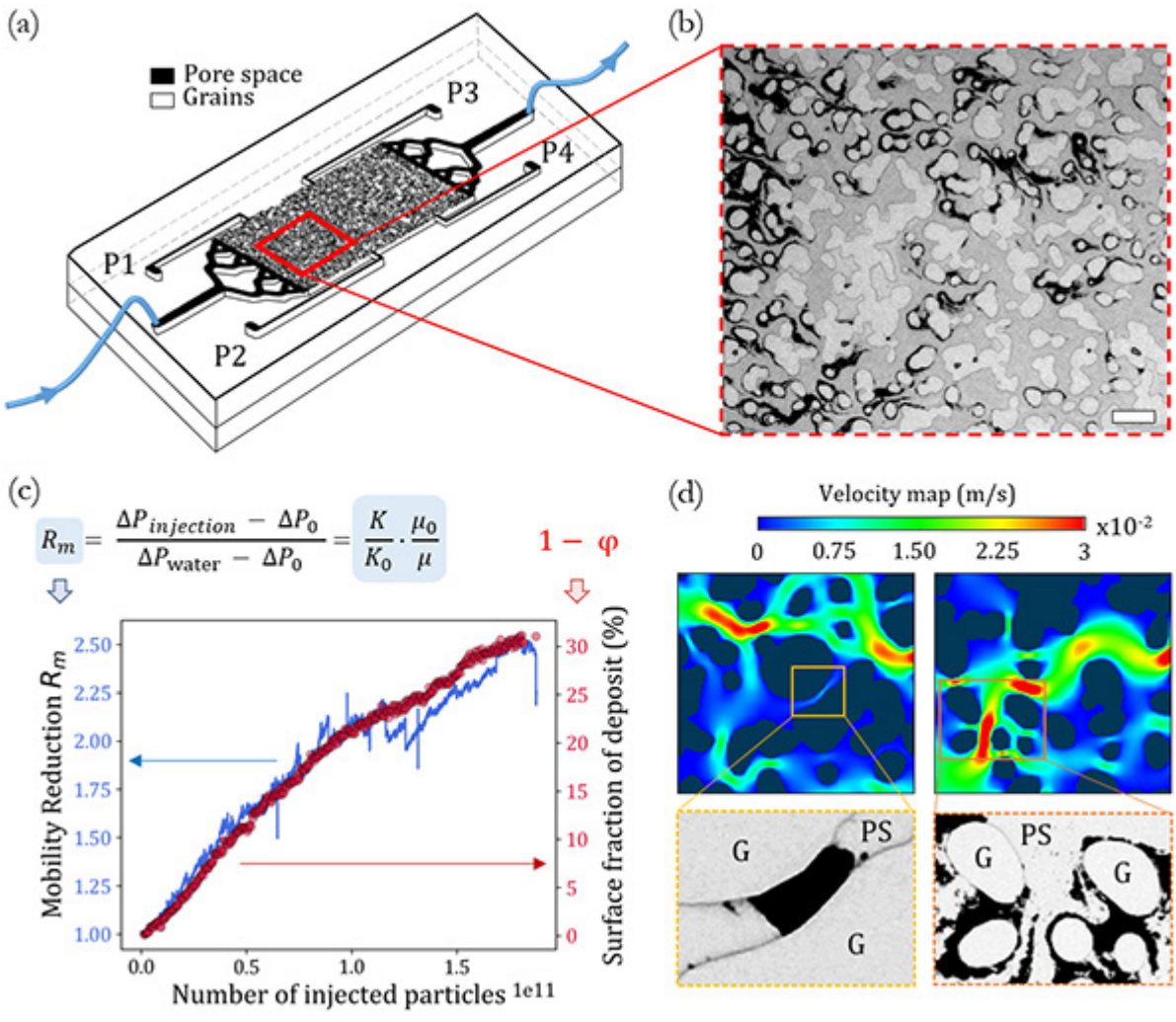

Figure 1:
(a) Illustration of the micromodel used. P1/P2/P3 and P4 correspond to pressure measurements.
(b) Example of observation based on traditional imaging of particle transport in porous media. The deposits, pore space and grains are shown in black, dark grey and light grey respectively. The scale bar corresponds to 850 µm.
(c) Characteristic evolution of the mobility reduction coefficient Rm during injection of a particulate suspension and of the associated porosity reduction, obtained via image processing.
(d) Local observations of deposition sites and nature as a function of location in the porous medium and local flow rate obtained by numerical simulation. G and PS correspond to a grain and the pore space respectively. The deposit is shown in black.

References:

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Microfluidics to understand and overcome geological clogging

Demeter Partners is a capital investment pioneer in the cleantech sector in France, Spain and Germany. What sort of companies and projects do you support?

Sophie Paturle: Since our creation in 2005, we have been supporting companies of all sizes, from start-ups whose innovation has barely left the laboratory, through to established SMEs. We also invest in infrastructures, enabling us to cover every type of need throughout the equity chain. Our aim is to transform innovative projects into profitable businesses. We are convinced that it is possible to play a positive role in the energy transition and the environment and run a profitable business at the same time. We have provided funding for 65 companies in10 years. Since each investment lasts for between 5 and 7 months, our portfolio evolves on a regular basis. Over the course of the last 6 months, we have invested in 10 start-ups, 4 development capital projects and 1 infrastructure project.

What are the needs of these companies and how do you address them?

S. P.: There are two types of needs and they vary depending on the company's stage of development. Firstly, of course, there are financial needs: start-up launch, growth of an SME, funding for a large infrastructure, etc. But additional support is also extremely important. For example, we might help a start-up put together a business plan, protect its industrial property and recruit, or assist an SME in the drawing up of a development and diversification strategy. Moreover, thanks to our pool of partners (investors, industrial players, competitiveness clusters, pubic authorities, etc.), we enable entrepreneurs to expand their network. Club Demeter meetings and themed events are organized throughout the year to this end.

IFPEN has been supporting Demeter Partners since its creation. What does this partnership bring you?

S. P.: That's right, IFPEN is a long-standing and leading partner: sponsor of the Demeter 1 fund, subscriber to successive funds and member of all our committees. We have developed close ties at every level, from research unit to general management. Its international influence and the partnerships it has forged have also helped us build a genuine cleantech eco-system. Its reputation also helps underpin the credibility of the companies we support when they seek new customers. In addition, IFPEN shares expert advice with consultative committees who examine projects for which we are considering providing funding support. Lastly, we draw on its intellectual property expertise to help entrepreneurs requiring guidance in this area.

Watch Sophie Paturle's interview (in French):

Three questions for Sophie Paturle, founding partner of the capital investment firm Demeter Partners.

Issue 56 of Science@ifpen - PhD projects and Yves Chauvin Prize
06 December 2024

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